L3 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:78071 CAPLUS
DOCUMENT NUMBER: 49:78071
ORIGINAL REFERENCE NO.: 49:14810g-i,14811a
TITLE: (5-Benzyloxy-3-indolyl)alkanamides
INVENTOR(S): Speeter, Merrill E.
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

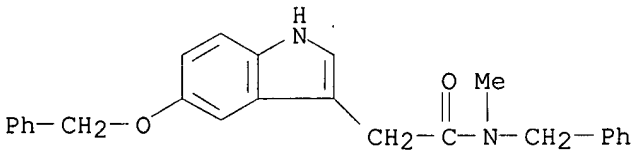
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2692882		19541026	US 1952-279931	19520401

GI For diagram(s), see printed CA Issue.

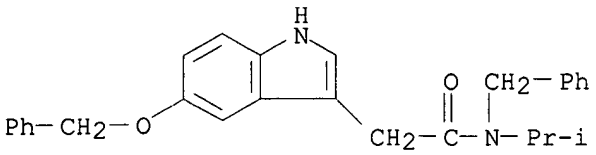
AB I (X is Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; Y is H, Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; R' and R'' are H or lower alkyl; n is 0 or 1; and Z is a secondary amine radical) are prepared by the following exemplary procedure. A Grignard reagent prepared from 4.25 g. MeI and 2.4 g. Mg in 200 ml. Et2O added to 5.5 g. 5-benzyloxyindole in 200 ml. Et2O, the solution refluxed 30 min., cooled in an ice-bath, 5.9 g. ClCH2CONMeCH2Ph in 200 ml. Et2O added, the mixture stirred, the Et2O distilled off, the residue warmed 3 hrs. on a steam bath, cooled, about 500 ml. Et2O added, then, with vigorous stirring, 5 ml. AcOH and 95 ml. H2O, the mixture allowed to stand overnight, and the product filtered and recrystd. gives 7.5 g. 2-(5-benzyloxy-3-indolyl)-N-benzyl-N-methylacetamide, m. 151-2° (from iso-PrOH). Similarly prepared: in 69% yield, the N,N-di-PhCH2 analog, m. 156-7°; and in 30% yield, 2-(5-benzyloxy-3-indolyl)benzylacetamide, m. 185-6°.

IT 725227-53-2P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- 857776-54-6P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- 857776-60-4P, 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- 872786-56-6P, Indole, 5-(benzyloxy)-3-(piperidinocarbonylmethyl)-
RL: PREP (Preparation)
(preparation of)

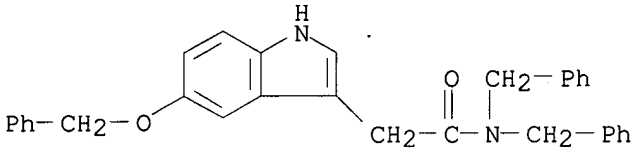
RN 725227-53-2 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- (5CI) (CA INDEX NAME)



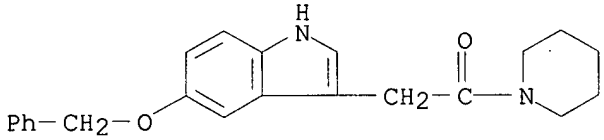
RN 857776-54-6 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- (5CI) (CA INDEX NAME)



RN 857776-60-4 CAPLUS
CN 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- (5CI) (CA INDEX NAME)



RN 872786-56-6 CAPLUS
CN Piperidine, 1-[[5-(benzyloxy)-3-indolyl]acetyl]- (5CI) (CA INDEX NAME)



Connecting via Winsock to STN

Claims 33-35

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 8	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS 10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS 11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS 12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 13	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 14	DEC 18	CA/CAplus patent kind codes updated
NEWS 15	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 17	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 19	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 22	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 23	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 24	JAN 29	PHAR reloaded with new search and display fields
NEWS 25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 26	FEB 13	CASREACT coverage to be extended
NEWS 27	Feb 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 28	Feb 15	RUSSIAPAT enhanced with pre-1994 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:12:58 ON 21 FEB 2007

=> fil casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CASREACT' ENTERED AT 16:13:04 ON 21 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 18 Feb 2007 VOL 146 ISS 8

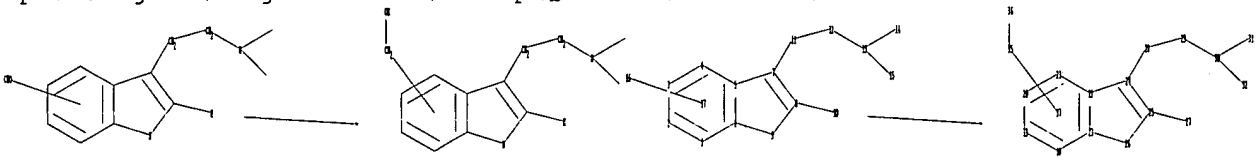
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 12 million reactions *
*
****

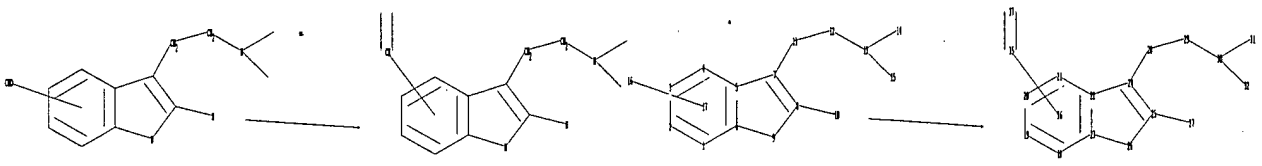
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 33.str



```
chain nodes :
10  11  12  16  27  28  29  35  36
ring nodes :
1  2  3  4  5  6  7  8  9  18  19  20  21  22  23  24  25  26
ring/chain nodes :
13  14  15  30  31  32
chain bonds :
7-11  8-10  11-12  12-13  24-28  25-27  28-29  29-30  35-36
ring/chain bonds :
13-14  13-15  30-31  30-32
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9  18-19  18-23  19-20  20-21  21-22
 22-23  22-24  23-26  24-25  25-26
exact/norm bonds :
5-7  6-9  7-8  8-9  13-14  13-15  22-24  23-26  24-25  25-26  30-31  30-32
exact bonds :
7-11  8-10  11-12  12-13  24-28  25-27  28-29  29-30  35-36
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  18-19  18-23  19-20  20-21  21-22  22-23


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:Atom  18:Atom
19:Atom  20:Atom  21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:CLASS
28:CLASS  29:CLASS  30:CLASS  31:CLASS  32:CLASS  35:CLASS  36:CLASS  37:Atom



L1      STRUCTURE UPLOADED

=>  d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
FULL SEARCH INITIATED 16:13:25 FILE 'CASREACT'
SCREENING COMPLETE -   102186 REACTIONS TO VERIFY FROM     5702 DOCUMENTS

100.0% DONE  102186 VERIFIED       0 HIT RXNS                        0 DOCS
SEARCH TIME: 00.00.05

L2            0 SEA SSS FUL L1 (     0 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 34.str
```



chain nodes :
10 11 12 16 27 28 29 35 37
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
13 14 15 30 31 32
chain bonds :
7-11 8-10 11-12 12-13 24-28 25-27 28-29 29-30 35-37
ring/chain bonds :
13-14 13-15 30-31 30-32
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20 20-21 21-22
22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15 22-24 23-26 24-25 25-26 30-31 30-32
exact bonds :
7-11 8-10 11-12 12-13 24-28 25-27 28-29 29-30 35-37
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 35:CLASS 36:Atom 37:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

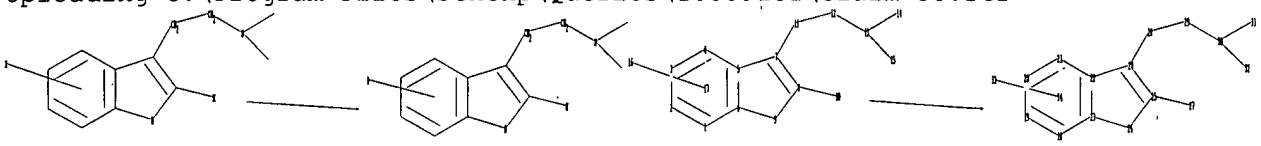
=> s l3 full
FULL SEARCH INITIATED 16:14:39 FILE 'CASREACT'
SCREENING COMPLETE - 21936 REACTIONS TO VERIFY FROM 1426 DOCUMENTS

100.0% DONE 21936 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L3 (0 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 35.str



chain nodes :
10 11 12 16 27 28 29 33
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
ring/chain nodes :
13 14 15 30 31 32
chain bonds :
7-11 8-10 11-12 12-13 24-28 25-27 28-29 29-30
ring/chain bonds :
13-14 13-15 30-31 30-32
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 18-19 18-23 19-20 20-21 21-22
22-23 22-24 23-26 24-25 25-26
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15 22-24 23-26 24-25 25-26 30-31 30-32
exact bonds :
7-11 8-10 11-12 12-13 24-28 25-27 28-29 29-30
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom
fragments assigned product role:
containing 18
fragments assigned reactant/reagent role:
containing 1

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> s l5 full
FULL SEARCH INITIATED 16:18:19 FILE 'CASREACT'
SCREENING COMPLETE -      168 REACTIONS TO VERIFY FROM       22 DOCUMENTS

100.0% DONE     168 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

L6            0 SEA SSS FUL L5 (     0 REACTIONS)

=>

---Logging off of STN---


=>
Executing the logoff script...


=> LOG Y

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   343.80     344.01

STN INTERNATIONAL LOGOFF AT 16:18:48 ON 21 FEB 2007
```

Connecting via Winsock to STN

Claim 36

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 8	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 9	DEC 01	CAS REGISTRY updated with new ambiguity codes
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NEWS 13	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
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NEWS 16	DEC 18	MEDLINE updated in preparation for 2007 reload
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NEWS 18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
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NEWS 20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 22	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 23	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 24	JAN 29	PHAR reloaded with new search and display fields
NEWS 25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 26	FEB 13	CASREACT coverage to be extended
NEWS 27	Feb 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 28	Feb 15	RUSSIAPAT enhanced with pre-1994 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:36:24 ON 21 FEB 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:36:28 ON 21 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 FEB 2007 HIGHEST RN 921921-74-6
DICTIONARY FILE UPDATES: 19 FEB 2007 HIGHEST RN 921921-74-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

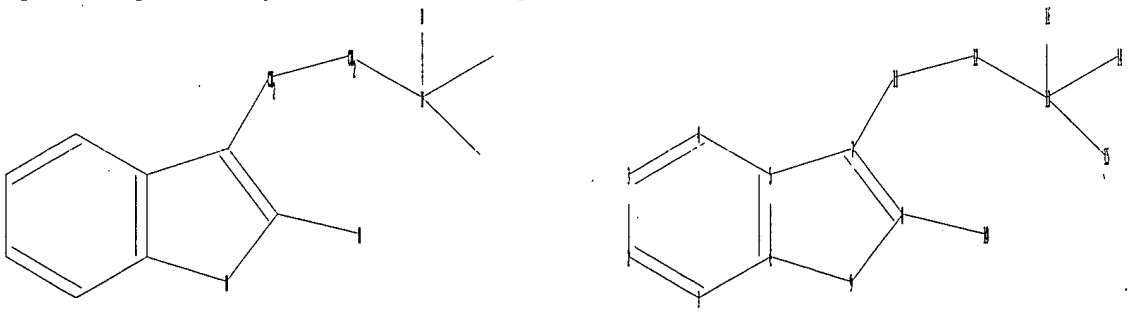
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 XIIIa.str



chain nodes :

```
10  11  12  16
ring nodes :
1  2  3  4  5  6  7  8  9
ring/chain nodes :
13  14  15
chain bonds :
7-11  8-10  11-12  12-13  13-16
ring/chain bonds :
13-14  13-15
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  13-14  13-15
exact bonds :
7-11  8-10  11-12  12-13  13-16
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS


L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
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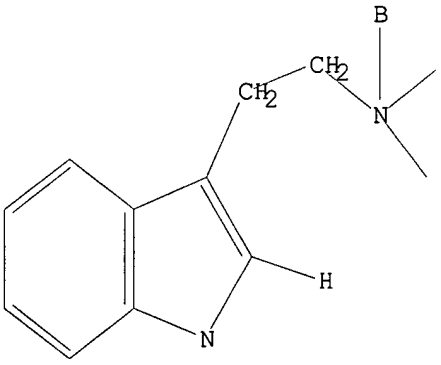


```
Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
FULL SEARCH INITIATED 16:36:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      164 TO ITERATE

100.0% PROCESSED      164 ITERATIONS                          8 ANSWERS
SEARCH TIME: 00.00.01

L2            8 SEA SSS FUL L1

=> fil caplus
```

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 16:36:47 ON 21 FEB 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 19 Feb 2007 (20070219/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

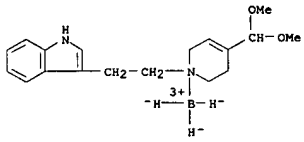
```
=> s l2
L3            7 L2

=> d ibib abs hitstr 1-7
```

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:465610 CAPLUS
DOCUMENT NUMBER: 127:176360
TITLE: Synthesis of 4-ethyloctahydroindolo[2,3-a]quinolizine-2-carbaldehydes
AUTHOR(S): Bonjoch, Josep; Fernandez, Joan-Carles; Terricabras, Dolors; Valls, Nativitat
CORPORATE SOURCE: Lab. Org. Chemistry, Fac. Pharmacy, Univ. Barcelona, Barcelona, 08028, Spain
SOURCE: Tetrahedron (1997), 53(27), 9407-9414
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:176360
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The isomerization-cyclization of tetrahydropyridine I by AcOH leads to 4-ethyloctahydroindolo[2,3-a]quinolizine-2-carbaldehydes II. When the process is carried out with aqueous AcOH, indolizidinoindole III is formed as a byproduct in a competitive way. Compound I is available via reductive cyanation of pyridinium salt IV followed by treatment of nitrile V with ethylmagnesium bromide.
IT 194086-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ethylindoloquinolizinecarbaldehydes)
RN 194086-75-4 CAPLUS
CN Boron, [3-[2-[4-(dimethoxymethyl)-3,6-dihydro-1(2H)-pyridinyl-κN]ethyl]-1H-indole]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:649833 CAPLUS
DOCUMENT NUMBER: 119:249833
TITLE: Indole derivatives which are potent serotinin receptor antagonists
INVENTOR(S): Macor, John E.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9311106	A1	19930610	WO 1992-US8306	19921006
W: AU, BR, CA, CS, DE, FI, HU, JP, KR, NO, PL, RU, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
AU 9228961	A	19930628	AU 1992-28961	19921006
AU 671959	B2	19960919		
EP 619805	A1	19941019	EP 1992-922831	19921006
EP 619805	B1	20000315		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE				
JP 06510793	T	19941201	JP 1992-510088	19921006
JP 2840448	B2	19981224		
HU 69705	A2	19950928	HU 1994-1398	19921006
BR 9206810	A	19951031	BR 1992-6810	19921006
CZ 281874	B6	19970312	CZ 1994-1280	19921006
PL 173875	B1	19980529	PL 1992-303794	19921006
RU 2126399	C1	19990220	RU 1994-28107	19921006
AT 190608	T	20000415	AT 1992-922831	19921006
ES 2143992	T3	20000601	ES 1992-922831	19921006
CA 2124206	C	20010227	CA 1992-2124206	19921006
IL 103798	A	20000813	IL 1992-103798	19921119
EG 21209	A	20010131	EG 1992-718	19921123
CN 1072679	A	19930602	CN 1992-113491	19921124
CN 1045294	B	19990929		
ZA 9209082	A	19940524	ZA 1992-9082	19921124
US 5639752	A	19970617	US 1994-244043	19940520
FI 9402395	A	19940524	FI 1994-2395	19940524
NO 9401918	A	19940524	NO 1994-1918	19940524
NO 301225	B1	19970929		
JP 08239363	A	19960917	JP 1996-38320	19960226
GR 3033370	T3	20000929	GR 2000-401055	20000505

PRIORITY APPLN. INFO.: US 1991-796744 A2 19911125
WO 1992-US8306 A 19921006

OTHER SOURCE(S): MARPAT 119:249833
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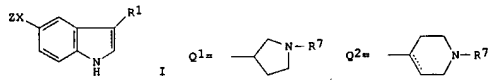
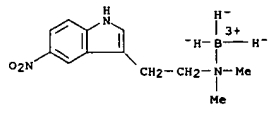
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. I [R1 = CH2CH2NR7R8, Q1, Q2 (dotted line represents an optional double bond), etc.; R7,R8 = H, C1-6alkyl, aryl, C1-3alkylaryl, etc.; X = O, NH, S; Z = (un)substituted 5- or 6-membered heterocycleo; R7R8 may form a 4- to 6-membered ring], which are potent serotonin (5-HT1) receptor antagonists (no data), useful in the treatment of hypertension (no data), depression (no data), anxiety (no data), eating disorders (no data), obesity (no data), etc., are prepared Thus, (R)-5-amino-3-(pyrrolidin-2-ylmethyl)-1-H-indole was prepared by hydrogenolysis of (R)-3-(N-benzyloxycarbonylpyrrolidin-2-ylmethyl)-5-dibenzylamino-1H-indole.
IT 147659-18-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of indole derivative serotonin receptor antagonists)
RN 147659-18-5 CAPLUS
CN Boron, (N,N-dimethyl-5-nitro-1H-indole-3-ethanamine-Nα)trihydro-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:233812 CAPLUS
DOCUMENT NUMBER: 118:233812
TITLE: A simple synthesis of 5-amino-3-(2-dimethylaminoethyl)indole [5-amino-N,N-dimethyltryptamine]
AUTHOR(S): Macor, John E.; Post, Ronald; Ryan, Kevin
CORPORATE SOURCE: Cent. Res. Div., Pfizer Inc., Groton, CT, 06355, USA
SOURCE: Synthetic Communications (1993), 23(1), 65-72
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:233812
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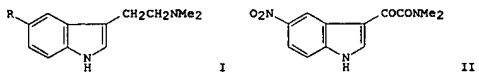
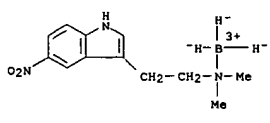


AB A short (three step) synthesis of the title compound (I, R = NH2) from com. available starting materials is presented. Reaction of 5-nitroindole with oxalyl chloride followed by dimethylamine afforded N,N-di-methyl-5-nitroindole-3-glyoxamide (II), which was reduced by diborane to 5-nitro-3-(2-dimethylaminoethyl)indole (I, R = NO2). Catalytic reduction of I (R = NO2) afforded the title compound in 19% overall yield from 5-nitroindole.
IT 147659-18-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomplexation of)
RN 147659-18-5 CAPLUS
CN Boron, (N,N-dimethyl-5-nitro-1H-indole-3-ethanamine-Nα)trihydro-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:174023 CAPLUS
DOCUMENT NUMBER: 116:174023
TITLE: The synthesis of pyrano[3,2-e]indoles and pyrano[2,3-f]indoles as rotationally restricted phenolic analogs of the neurotransmitter serotonin
AUTHOR(S): Macro, John E.; Ryan, Kevin; Newman, Michael E.
CORPORATE SOURCE: Cent. Res. Div., Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Tetrahedron (1992), 48(6), 1039-52
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
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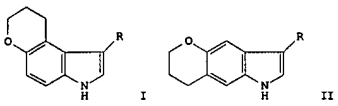
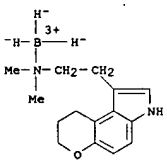


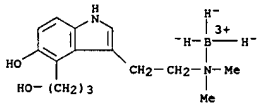
I II

AB The synthesis of two rotationally restricted phenolic analogs I and II (R = CH2CH2NMe2) of the neurotransmitter serotonin have been accomplished. The syntheses of dihydropyranoindoles I and II (R = H), which formed the template for these targets, are outlined. These novel fused-indoles represent rotationally restricted phenolic analogs of 5-hydroxyindole. The reaction sequence of Claisen rearrangement of 3-Me,4-(NO2)C6H3OCH2CH:CH2, followed by olefin hydroxylation, and intramol. Mitsunobu reaction was used to form the fused dihydropyran rings.
IT 135530-03-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 135530-03-9 CAPLUS
CN Boron, trihydro(3,7,8,9-tetrahydro-N,N-dimethylpyrano[3,2-e]indole-1-ethanamine-Nα)-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 135530-02-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. Mitsunobu reaction of)
RN 135530-02-8 CAPLUS
CN Boron, [3-[2-(dimethylamino)ethyl]-5-hydroxy-1H-indole-4-propanol-N3]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:492116 CAPLUS
DOCUMENT NUMBER: 115:92116
TITLE: Synthesis of a dihydropyrano[3,2-e]indole as a rotationally restricted phenolic analog of the neurotransmitter serotonin
AUTHOR(S): Macor, John E.; Newman, Michael E.
CORPORATE SOURCE: Cent. Res. Div., Pfizer, Inc., Groton, CT, 06340, USA
SOURCE: Tetrahedron Letters (1991), 32(28), 3345-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:92116
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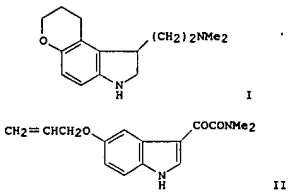
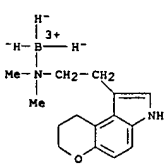
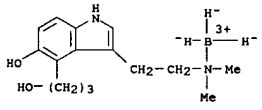


I II

AB Dihydropyranoindole I has been synthesized via a six step procedure involving a Claisen rearrangement of allyloxyindoleglyoxamide II. The novel heterocycle I represents a rotationally restricted phenolic analog of the neurotransmitter serotonin [3-(2-aminoethyl)-5-hydroxyindole].
IT 135530-03-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 135530-03-9 CAPLUS
CN Boron, trihydro(3,7,8,9-tetrahydro-N,N-dimethylpyrano[3,2-e]indole-1-ethanamine-Nα)-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 135530-02-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. Mitsunobu reaction of)
RN 135530-02-8 CAPLUS
CN Boron, [3-[2-(dimethylamino)ethyl]-5-hydroxy-1H-indole-4-propanol-N3]trihydro-, (T-4)- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:199969 CAPLUS
DOCUMENT NUMBER: 96:199969
TITLE: The partial syntheses of reserpiline and isoreserpiline
AUTHOR(S): Sakai, Shinichiro; Saito, Naoki; Hirose, Naohiro; Yamanaka, Etsuji
CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, 260, Japan
SOURCE: Heterocycles (1982), 17(Spec. Issue), 99-103
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
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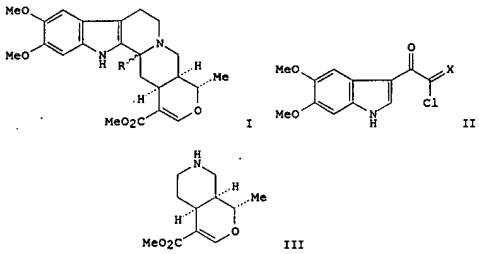
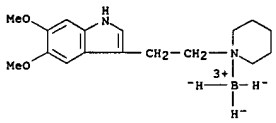


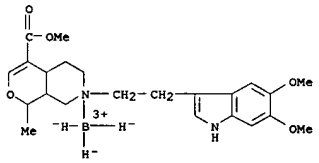
I II III

AB Reserpiline (I, R = β-H) and isoreserpiline (I, R = α-H) were synthesized through 5,6-dimethoxyindole derivative II (X = H2, O) and amine
synthon III which was already derived from natural oxindole alkaloids and/or by the total syntheses.
IT 81641-54-5P 81642-36-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81641-54-5 CAPLUS
CN Boron, [5,6-dimethoxy-3-[2-(1-piperidinyl)ethyl]-1H-indole-N3]trihydro-, (T-4)- (9CI) (CA INDEX NAME)

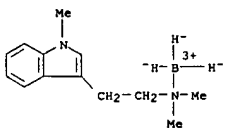
L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 81642-36-6 CAPLUS
CN Boron, trihydro[methyl 7-[2-(5,6-dimethoxy-1H-indol-3-yl)ethyl]-4a,5,6,7,8,8a-hexahydro-1-methyl-1H-pyrano[3,4-c]pyridine-4-carboxylate]-, [T-4-[1R-(1α,4aα,8aα)]]- (9CI) (CA INDEX NAME)

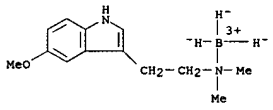


L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:147723 CAPLUS
DOCUMENT NUMBER: 78:147723
TITLE: Comparison of lithium aluminum hydride and diborane in
the reduction of certain 3-indolylglyoxamides
AUTHOR(S): Littell, Ruddy; Allen, George R., Jr.
CORPORATE SOURCE: Lederle Lab. Div., Am. Cyanamid Co., Pearl River, NY, USA
SOURCE: Journal of Organic Chemistry (1973), 38(8), 1504-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The utility of LiAlH4 and diborane for the preparation of trypthamines fro
3-indolylglyoxamides, including 4-trifluoromethyl derivs., was studied. Diborane allows elaboration of the tryptamine, side-chain without concomitant reduction of trifluoromethyl substituents, whereas these groups
are converted into Me substituents by LiAlH4 when reducing conditions are sufficiently vigorous to give the tryptamine. Reduction of the glyoxamides
with diborane may be accompanied by reduction of th indolic enamine triad to
give indolines, an event not seen with LiAlH4. 1-Alkyl-3-indolyglyoxamides are converted into the corresponding trypta- mines by diborane, whereas LiAlH reduction gives 1-alkyl-3-indolylglyco- lamines. The
formation of a 3,4,5,6-tetrahydro-1H-azepino[5,4,3-cd]indole was observed in the LiAlH4 reduction of 5-methoxy-N,N,2-trimethyl-4-(trifluoromethyl)-3-
indolylglyoxamide. Diborane reduction of 3-indolecarboxylic acid and its ethyl
ester gave skatole as the major product.
IT 38662-20-3P 38662-23-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38662-20-3 CAPLUS
CN Boron, trihydro(N,N,1-trimethyl-1H-indole-3-ethanamine-Nα)-, (T-4)- (9CI) (CA INDEX NAME)



RN 38662-23-6 CAPLUS
CN Boron, trihydro(5-methoxy-N,N-dimethyl-1H-indole-3-ethanamine-Nα)-, (T-4)- (9CI) (CA INDEX NAME)

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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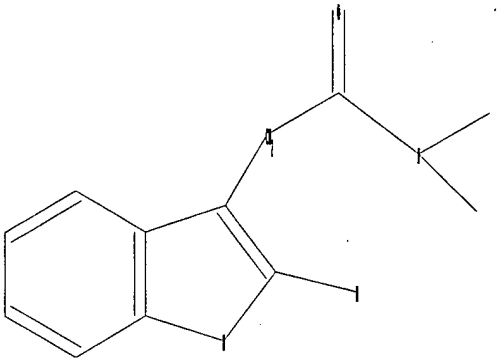

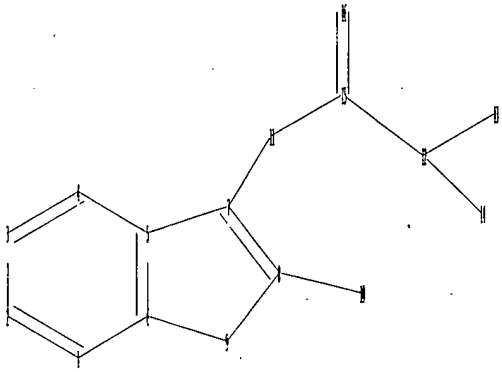

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Match level :
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L4 STRUCTURE UPLOADED

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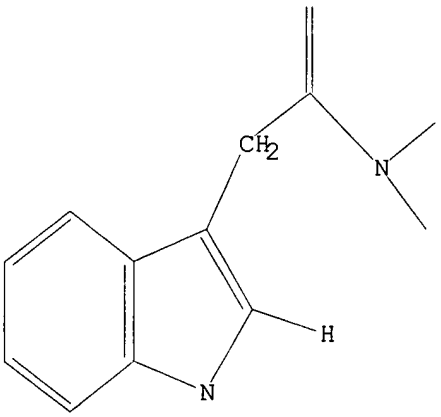

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L6 309 L5

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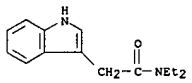
L6 ANSWER 309 OF 309 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1938:6240 CAPLUS
DOCUMENT NUMBER: 32:6240
ORIGINAL REFERENCE NO.: 32:939e-g
TITLE: Diethylamide of the indole-3-carboxylic acid, β-indole-acetic acid, thionaphthene-3-carboxylic acid, and of the hydrogenated β-indolylacetic acid
AUTHOR(S): Wegler, Richard; Binder, Hans
SOURCE: Arch. Pharm. (1937), 275, 506-16
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The following compds. were prepared and characterized: di-ethylamide of indolyl-3-carboxylic acid by interaction of Mg, MeI and indole, thereupon treatment of the resulting indolylmagnesium iodide with Et2NCOCl, C13H16ON2, m. 151-1.5° (picrate m. 129.5-30°); diethylamide of thionaphthene-3-carboxylic acid, C13H15ONS, oil, b11 220°; amide of indole-3-carboxylic acid, m. 200°; diethylamide of β-indolylacetic acid, C14H18ON, m. 101° (picrate m. 139-40°); β-indolylacetamide; diethylamide of 2,3-dihydro- and octahydro-3-indolylacetic acid (picrate of the dihydro compound m. 170-2°; salt of 2-nitro-1,3-diketohydrindene, yellow, m. 184°); picrate of the octahydro compound yellow, m. 177-8.5°); diethylamide of N-nitrosoindolyl-3-carboxylic acid, C13H15O2N3, m. 241-2°; diethylamide of N-aminoindolyl-3-carboxylic acid, C13H17ON3 m. 177.5-8°.
IT 100722-27-8P, 3-Indoleacetamide, N,N-diethyl- 859965-26-7P , 3-Indoleacetamide, N,N-diethyl-, picrate
RL: PREP (Preparation)
(preparation of)
RN 100722-27-8 CAPLUS
CN 1H-Indole-3-acetamide, N,N-diethyl- (9CI) (CA INDEX NAME)



RN 859965-26-7 CAPLUS
CN 3-Indoleacetamide, N,N-diethyl-, picrate (4CI) (CA INDEX NAME)

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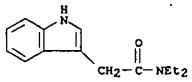
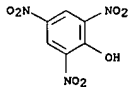
CRN 100722-27-8
CMF C14 H18 N2 O



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



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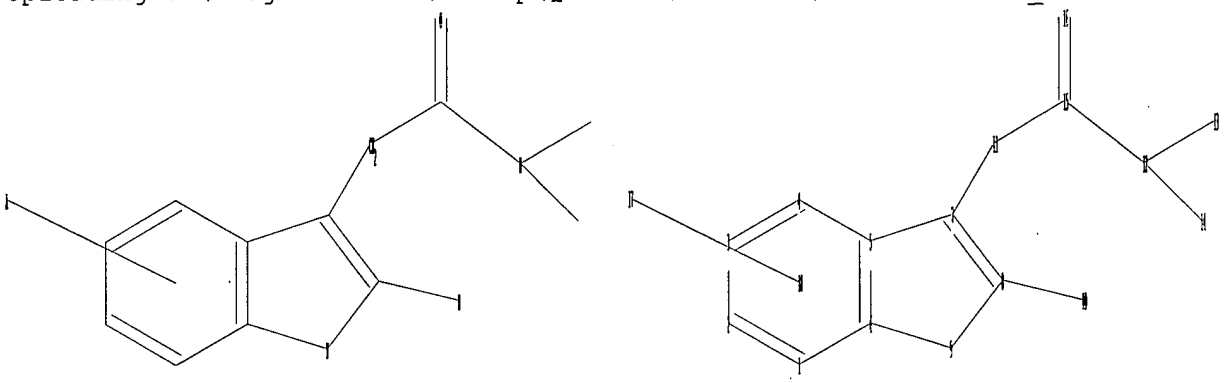

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ring nodes :
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ring/chain nodes :
12 13 14
chain bonds :
7-11 8-10 11-15 12-15 15-16
ring/chain bonds :
12-14 12-13
ring bonds :
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Match level :
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11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom

L7 STRUCTURE UPLOADED

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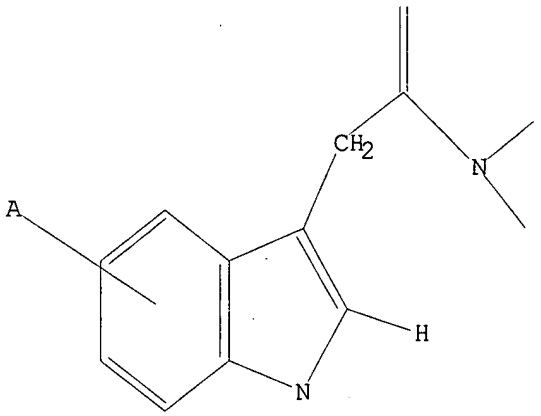
L7 HAS NO ANSWERS
L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l7 full sub=l5
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 16:40:51 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 826 TO ITERATE

100.0% PROCESSED 826 ITERATIONS 122 ANSWERS
SEARCH TIME: 00.00.01

L8 122 SEA SUB=L5 SSS FUL L7

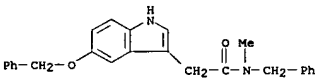
SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH
L9 69 L8

=> d ibib abs hitstr 69

L9 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:78071 CAPLUS
DOCUMENT NUMBER: 49:78071
ORIGINAL REFERENCE NO.: 49:14810g-i,14811a
TITLE: (5-Benzyloxy-3-indolyl)alkanamides
INVENTOR(S): Speeter, Merrill E.
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

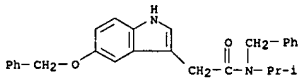
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2692882		19541026	US 1952-279931	19520401

GI For diagram(s), see printed CA Issue.
AB I (X is Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; Y is H, Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; R' and R'' are H or lower alkyl; n is 0 or 1; and Z is a secondary amine radical) are prepared by the following exemplary procedure. A Grignard reagent prepared from 4.25 g. MeI and 2.4 g. Mg in 200 ml. Et2O added to 5.5 g. 5-benzyloxyindole in 200 ml. Et2O, the solution refluxed 30 min., cooled in an ice-bath, 5.9 g. ClCH2CONMeCH2Ph in 200 ml. Et2O added, the mixture stirred, the Et2O distilled off, the residue warmed 3 hrs. on a steam bath, cooled, about 500 ml. Et2O added, then, with vigorous stirring, 5 ml. AcOH and 95 ml. H2O, the mixture allowed to stand overnight, and the product filtered and recrystd. gives 7.5 g. 2-(5-benzyloxy-3-indolyl)-N-benzyl-N-methylacetamide, m. 151-2° (from iso-PrOH). Similarly prepared: in 69% yield, the N,N-di-PhCH2 analog, m. 156-7°; and in 30% yield, 2-(5-benzyloxy-3-indolyl)benzylacetamide, m. 185-6°.
IT 725227-53-2P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- 857776-54-6P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- 857776-60-4P, 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- 872786-56-6P, Indole, 5-(benzyloxy)-3-(piperidinocarbonylmethyl)-
RL: PREP (Preparation)
(preparation of)
RN 725227-53-2 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- (5CI) (CA INDEX NAME)

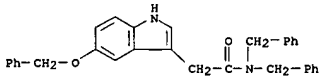


RN 857776-54-6 CAPLUS

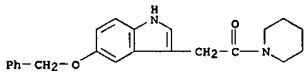
L9 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- (5CI) (CA INDEX NAME)



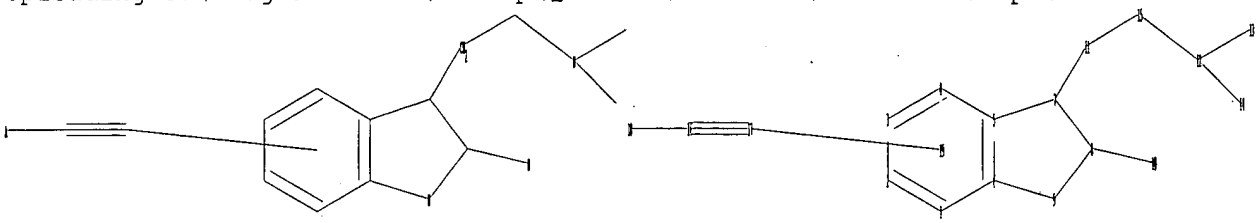
RN 857776-60-4 CAPLUS
CN 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- (5CI) (CA INDEX NAME)



RN 872786-56-6 CAPLUS
CN Piperidine, 1-[[5-(benzyloxy)-3-indolyl]acetyl]- (5CI) (CA INDEX NAME)



=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 triple bond.str

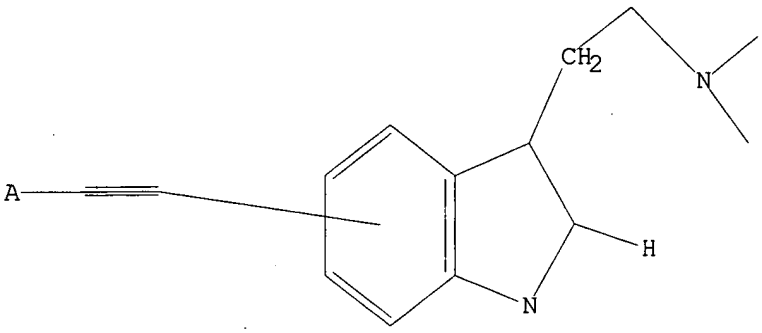


chain nodes :
10 11 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
12 13 14
chain bonds :
7-11 8-10 11-15 12-15 16-17 16-18
ring/chain bonds :
12-14 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 12-14 12-13 12-15 16-18
exact bonds :
7-11 8-10 11-15 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:Atom

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

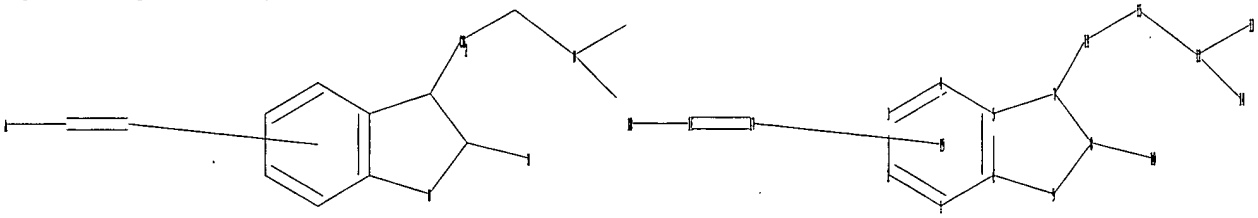
FULL SEARCH INITIATED 16:47:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1115 TO ITERATE

100.0% PROCESSED 1115 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L10

L12 0 L11

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 double bond.str



chain nodes :
10 11 15 16 17 18
ring nodes :

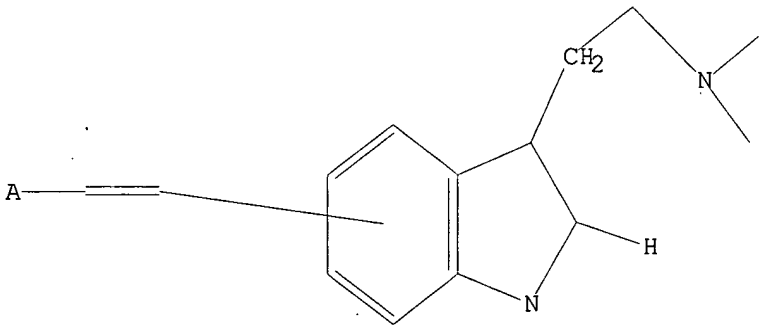
```
1  2  3  4  5  6  7  8  9
ring/chain nodes :
12  13  14
chain bonds :
7-11  8-10  11-15  12-15  16-17  16-18
ring/chain bonds :
12-14  12-13
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  12-14  12-13  12-15  16-18
exact bonds :
7-11  8-10  11-15  16-17
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS
19:Atom



L13     STRUCTURE UPLOADED

=>  d
L13 HAS NO ANSWERS
L13             STR
```

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Structure attributes must be viewed using STN Express query preparation.


=> s l13 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

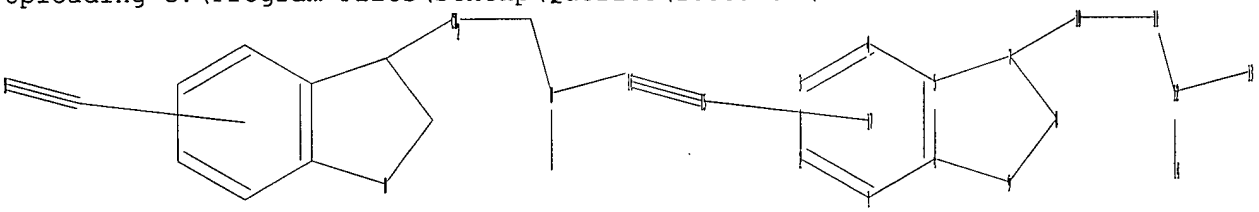
FULL SEARCH INITIATED 16:48:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17377 TO ITERATE

100.0% PROCESSED 17377 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L14 0 SEA SSS FUL L13

L15 0 L14

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 CN.str

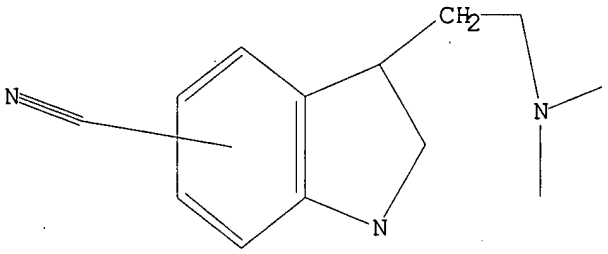


chain nodes :
10 11 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
12 13 14
chain bonds :
7-10 10-11 11-12 15-16
ring/chain bonds :
12-13 12-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 11-12 12-13 12-14 15-16
exact bonds :
7-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L16 STRUCTURE UPLOADED

=> d
L16 HAS NO ANSWERS
L16 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l16 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 16:53:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10023 TO ITERATE

100.0% PROCESSED 10023 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

L17 9 SEA SSS FUL L16

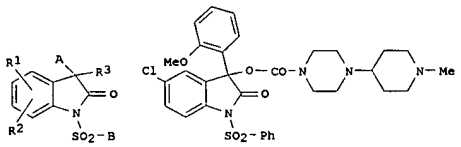
L18 1 L17

=> d ibib abs hitstr L18

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:54890 CAPLUS
DOCUMENT NUMBER: 144:150235
TITLE: Preparation of 1,3-dihydro-1-(phenylsulfonyl)-2H-indol-2-ones and related compounds as vasopressin V1B receptor modulators
INVENTOR(S): Lubisch, Wilfried; Oost, Thorsten; Wernet, Wolfgang; Unger, Liliane; Hornberger, Wilfried; Geneste, Herve
PATENT ASSIGNEE(S): Abbott Gmbh & Co.Kg, Germany
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006005609	A2	20060119	WO 2005-EP7631	20050713
WO 2006005609	A3	20060316		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004033834	A1	20060202	DE 2004-102004033834	20040713
PRIORITY APPLN. INFO.:			DE 2004-102004033834A	20040713
			US 2004-587407P P	20040713

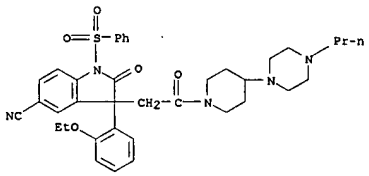
OTHER SOURCE(S): MARPAT 144:150235
GI



I II

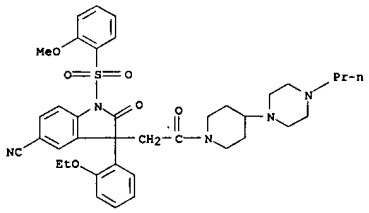
L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Title compds. I [A = (un)substituted aryl; B = (un)substituted aromatic, etc.; R1 = H, alkyl, OH, etc.; R2 = H, alkyl, O-alkyl, etc.; R3 = -Z-Y-X-W; W = alkylene, alkylene-O-alkylene, etc.; X = CO, SO2, C=NH, etc.; Y = pyrrolidinyl, pyridinyl, azepanyl, etc.] and their pharmaceutically acceptable salts were prepared For example, phenylsulfonylindolone II was prepared from 5-chloroisatin in 4-steps. In vasopressin V1B receptor binding assays, 9-examples of compds. I exhibited Ki values <100 nM.
IT 873955-53-4P 873955-54-5P 873955-55-6P 873955-56-7P 873955-57-8P 873955-58-9P 873955-59-0P 873955-71-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylsulfonylindolones and related compds. for the treatment of vasopressin or oxytocin dependent diseases)
RN 873955-53-4 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-2,3-dihydro-2-oxo-1-(phenylsulfonyl)-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

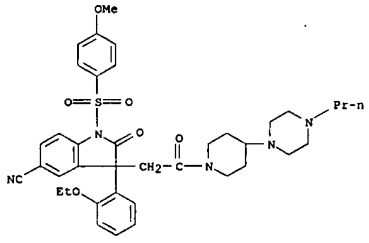


RN 873955-54-5 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-2,3-dihydro-1-[(2-methoxyphenyl)sulfonyl]-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

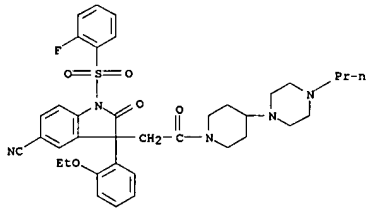


RN 873955-55-6 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-2,3-dihydro-1-[(4-methoxyphenyl)sulfonyl]-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

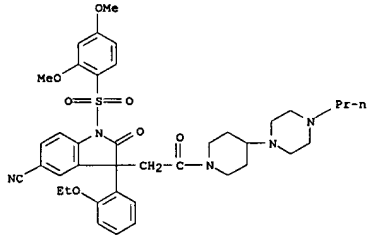


RN 873955-56-7 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-1-[(2-fluorophenyl)sulfonyl]-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

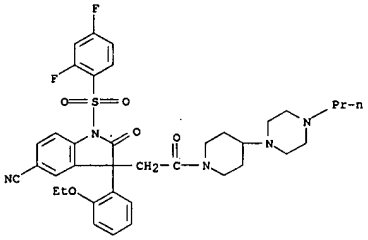


RN 873955-57-8 CAPLUS
CN Piperidine, 1-[[5-cyano-1-[(2,4-dimethoxyphenyl)sulfonyl]-3-(2-ethoxyphenyl)-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

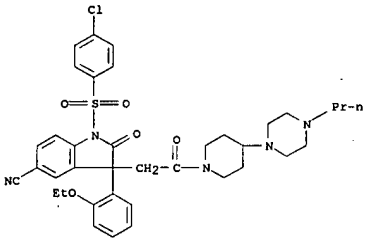


RN 873955-58-9 CAPLUS
CN Piperidine, 1-[[5-cyano-1-[(2,4-difluorophenyl)sulfonyl]-3-(2-ethoxyphenyl)-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

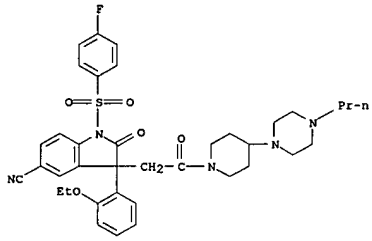


RN 873955-59-0 CAPLUS
CN Piperidine, 1-[[1-[(4-chlorophenyl)sulfonyl]-5-cyano-3-(2-ethoxyphenyl)-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

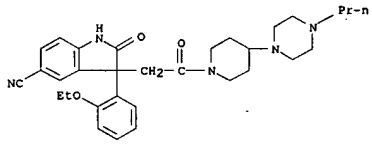


RN 873955-71-6 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-1-[(4-fluorophenyl)sulfonyl]-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

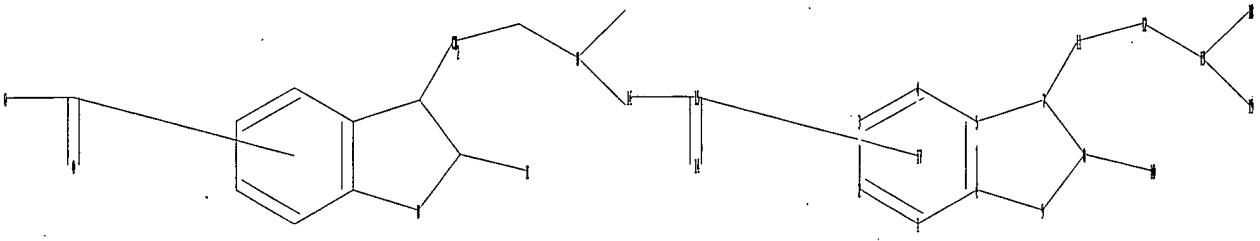
L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 873955-87-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylsulfonylindolones and related compds. for the treatment of vasopressin or oxytocin dependent diseases)
RN 873955-87-4 CAPLUS
CN Piperidine, 1-[[5-cyano-3-(2-ethoxyphenyl)-2,3-dihydro-2-oxo-1H-indol-3-yl]acetyl]-4-(4-propyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 ester.str



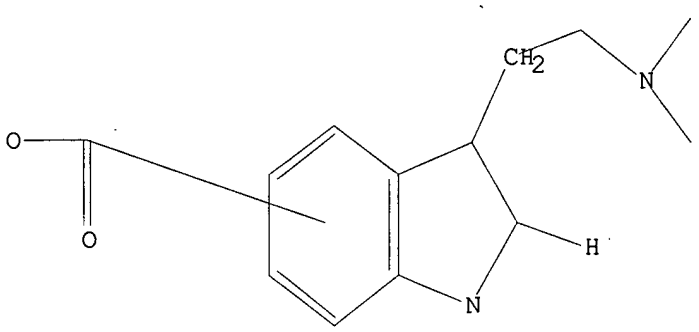
chain nodes :
10 11 12 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 18 19
chain bonds :
7-11 8-10 11-12 12-13 14-15 15-16
ring/chain bonds :
13-18 13-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 12-13 13-18 13-19 14-15 15-16
exact bonds :
7-11 8-10 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:CLASS
19:CLASS

L19 STRUCTURE UPLOADED

=> d
L19 HAS NO ANSWERS
L19 STR



G1 H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l19 full
   REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:00:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 325244 TO ITERATE

100.0% PROCESSED 325244 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.02

L20 3 SEA SSS FUL L19

L21 1 L20

=> d ibib abs histr
'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM

IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):ibib

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:322670 CAPLUS
DOCUMENT NUMBER: 135:122435
TITLE: A novel series of thromboxane A2 synthetase inhibitors with free radical scavenging and anti-peroxidative activities
AUTHOR(S): Kamiya, Shoji; Shirahase, Hiroaki; Nakamura, Shohei; Kanda, Mamoru; Matsui, Hiroshi; Yoshimi, Akihisa; Kasai, Masayasu; Takahashi, Kenji; Kurahashi, Kazuyoshi
CORPORATE SOURCE: Research Laboratories, Kyoto Pharmaceutical Industries, Ltd., Kyoto, 604-8444, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(5), 563-571
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122435
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

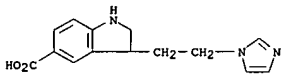
=> d ibib abs hitstr L21

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:322670 CAPLUS
DOCUMENT NUMBER: 135:122435
TITLE: A novel series of thromboxane A2 synthetase inhibitors with free radical scavenging and anti-peroxidative activities
AUTHOR(S): Kamiya, Shoji; Shirahase, Hiroaki; Nakamura, Shohei; Kanda, Mamoru; Matsui, Hiroshi; Yoshimi, Akihisa; Kasai, Masayasu; Takahashi, Kenji; Kurahashi, Kazuyoshi
CORPORATE SOURCE: Research Laboratories, Kyoto Pharmaceutical Industries, Ltd., Kyoto, 604-8444, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(5), 563-571
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122435

AB A novel series of indoline derivs. with imidazole and carboxyl moieties were synthesized and evaluated for their thromboxane A2 (TXA2) synthetase inhibiting, radical scavenging and anti-peroxidative activities. Among the compds. synthesized, 3-[5-substituted-3-[2-(imidazol-1-yl)ethyl]indolin-1-yl]propionic acids showed free radical scavenging activity and inhibitory effects on lipid-peroxidn. of rat brain homogenate and on arachidonate-induced TXA2-dependent aggregation of rabbit platelets. The anti-platelet and anti-peroxidative activities were related to the lipophilicity of the 5-substituent. The 5-hexyloxy derivative (I) showed about 35-fold higher inhibitory activity on TXA2 synthesis than that of ozagrel and about 100-fold higher activity on lipid peroxidn. than that of α-tocopherol. Compound I showed in vivo anti-thrombotic effect in mice and ex vivo anti-peroxidative activity in rats.

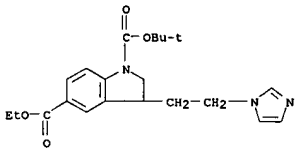
IT 350683-18-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of indoline thromboxane A2 synthetase inhibitors with free radical scavenging and anti-peroxidative activities)
RN 350683-18-0 CAPLUS
CN 1H-Indole-5-carboxylic acid, 2,3-dihydro-3-[2-(1H-imidazol-1-yl)ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



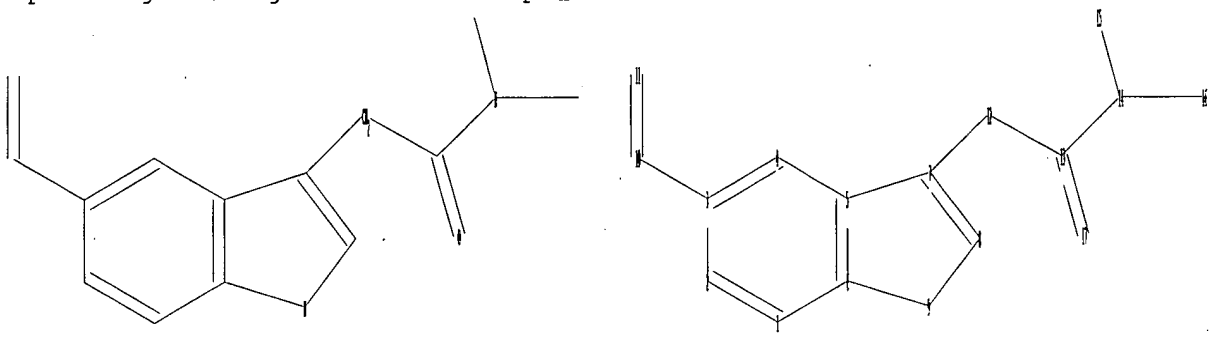
●2 HCl

IT 350683-34-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indoline thromboxane A2 synthetase inhibitors with free radical scavenging and anti-peroxidative activities)
RN 350683-34-0 CAPLUS
CN 1H-Indole-1,5-dicarboxylic acid, 2,3-dihydro-3-[2-(1H-imidazol-1-yl)ethyl]-, 1-(1,1-dimethylethyl) 5-ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 XXI.str

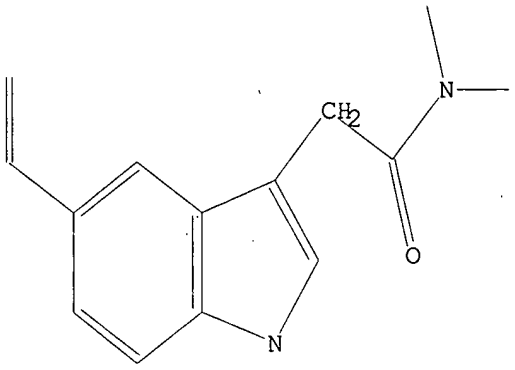


chain nodes :
10 11 12 13 17
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
14 15 16
chain bonds :
3-10 7-12 10-11 12-13 13-14 13-17
ring/chain bonds :
14-15 14-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-17 14-15 14-16
exact bonds :
3-10 7-12 10-11 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L22 STRUCTURE UPLOADED

=> d
L22 HAS NO ANSWERS
L22 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l22 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

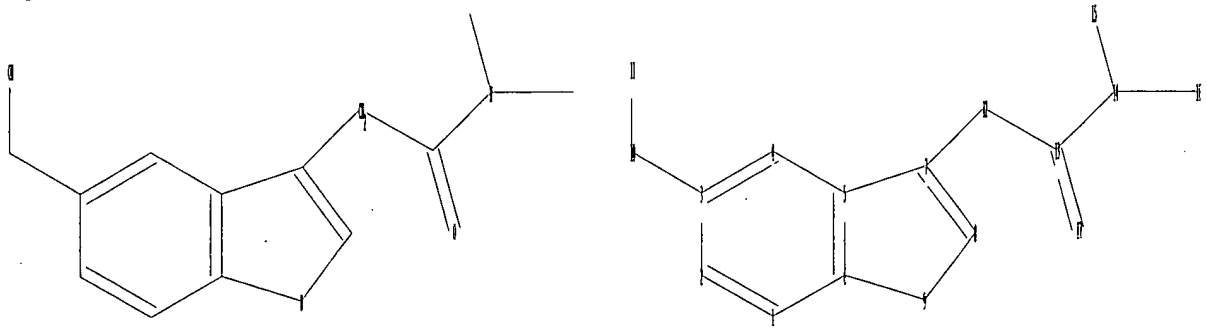
FULL SEARCH INITIATED 17:03:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 668 TO ITERATE

100.0% PROCESSED 668 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L23 0 SEA SSS FUL L22

L24 0 L23

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 35 XXIstarstar.str



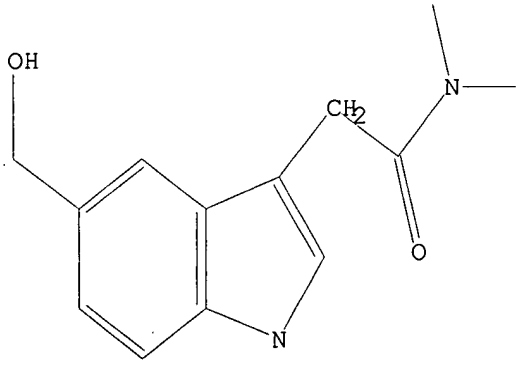
chain nodes :

```
10  11  12  13  17
ring nodes :
1  2  3  4  5  6  7  8  9
ring/chain nodes :
14  15  16
chain bonds :
3-10  7-12  10-11  12-13  13-14  13-17
ring/chain bonds :
14-15  14-16
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  10-11  13-14  13-17  14-15  14-16
exact bonds :
3-10  7-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS

L25     STRUCTURE UPLOADED

=>  d
L25 HAS NO ANSWERS
L25             STR
```




```
Structure attributes must be viewed using STN Express query preparation.

=> s l25 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

FULL SEARCH INITIATED 17:04:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11168 TO ITERATE

100.0% PROCESSED 11168 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L26 3 SEA SSS FUL L25

L27 1 L26

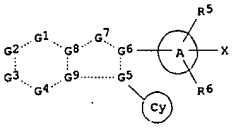
=> d ibib abs hitstr

L27 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:141029 CAPLUS
DOCUMENT NUMBER: 142:240430
TITLE: Preparation of heterocyclic compounds as hepatitis C virus polymerase inhibitors
INVENTOR(S): Oka, Takahiro; Yata, Shinji; Ikegashira, Kazutaka; Noji, Satoru; Akaki, Tatsuo; Hirashima, Shintaro; Niwa, Yasushi; Ando, Izuru; Sato, Toshihiro
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 467 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014543	A1	20050217	WO 2004-JP11640	20040806
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 2003-288296 A 20030806
JP 2003-288298 A 20030806

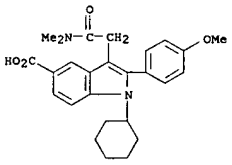
OTHER SOURCE(S): MARPAT 142:240430
GI



I

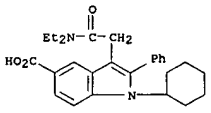
AB The title compds. I [G1 = CR1, N; G2 = CR2, N; G3 = CR3, N; G4 = CR4, N; G5, G6,G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, halo, etc.; R5, R6 = H, halo, etc.; ring Cy = (un)substituted cycloalkyl, etc.; ring A = aryl, etc.; X = H, halo, etc.] are prepared Thus, 2-[4-[2-(4-chlorophenyl)-5-(2-oxopyrrolidin-1-yl)benzyloxy]phenyl]-3-cyclohexyl-1-methyl-1-H-indole-6-

L27 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

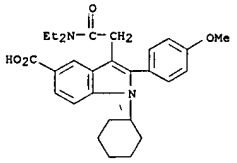


REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L27 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
carboxylic acid was prepd. in a multistep process starting from Me 3-aminobenzoate. In an in vitro test for hepatitis C virus polymerase inhibiting activity, compds. of this invention showed IC50 values of < 0.01 μM to < 1 μM. Formulations are given.
IT 844895-87-0P 844895-88-1P 844895-90-5P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. as hepatitis C virus polymerase inhibitors)
RN 844895-87-0 CAPLUS
CN 1H-Indole-5-carboxylic acid, 1-cyclohexyl-3-[2-(diethylamino)-2-oxoethyl]-2-phenyl- (9CI) (CA INDEX NAME)

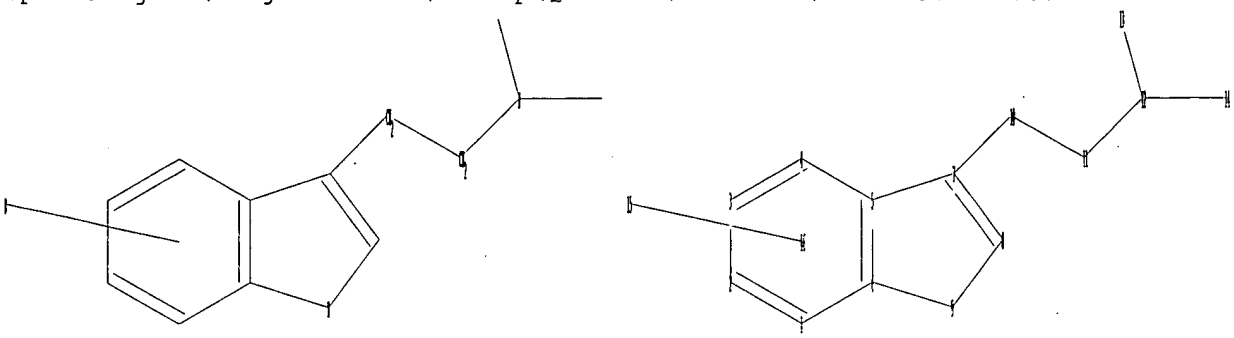


RN 844895-88-1 CAPLUS
CN 1H-Indole-5-carboxylic acid, 1-cyclohexyl-3-[2-(diethylamino)-2-oxoethyl]-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 844895-90-5 CAPLUS
CN 1H-Indole-5-carboxylic acid, 1-cyclohexyl-3-[2-(dimethylamino)-2-oxoethyl]-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 36 XX7.str

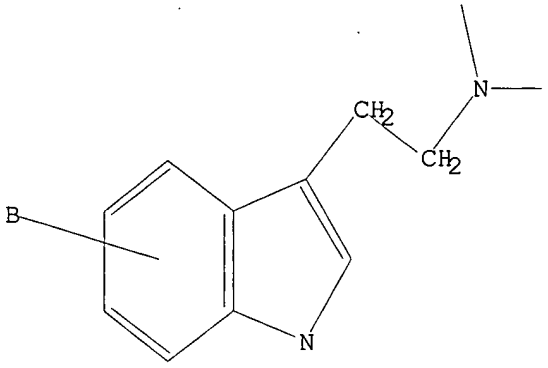


chain nodes :
10 11 15
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
12 13 14
chain bonds :
7-10 10-11 11-12
ring/chain bonds :
12-13 12-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 12-13 12-14
exact bonds :
7-10 10-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom

L28 STRUCTURE UPLOADED

=> d
L28 HAS NO ANSWERS
L28 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l28 full
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:05:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 257 TO ITERATE

100.0% PROCESSED 257 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L29 0 SEA SSS FUL L28

L30 0 L29

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.47	1677.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.36

STN INTERNATIONAL LOGOFF AT 17:06:02 ON 21 FEB 2007

STN - Cas react

Claim 24

chain nodes :
10 11 12 25 26 27 31 32 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 22 23 24
ring/chain nodes :
13 14 15 28 29 30
chain bonds :
7-11 8-10 9-31 11-12 12-13 22-26 23-25 24-32 26-27 27-28 33-34
ring/chain bonds :
13-14 13-15 28-29 28-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-20
20-21 20-22 21-24 22-23 23-24
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15 20-22 21-24 22-23 23-24 24-32 28-29 28-30
33-34
exact bonds :
7-11 8-10 9-31 11-12 12-13 22-26 23-25 26-27 27-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

G1:Si,Cb,Ak,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1
node mappings:

9:24 8:23 7:22 5:20 6:21

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

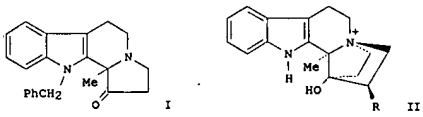
=> s l1 full
FULL SEARCH INITIATED 10:07:00 FILE 'CASREACT'
SCREENING COMPLETE - 45295 REACTIONS TO VERIFY FROM 3761 DOCUMENTS

100.0% DONE 45295 VERIFIED 111 HIT RXNS 31 DOCS
SEARCH TIME: 00.00.05

L2 31 SEA SSS FUL L1 (111 REACTIONS)

=> d ibib abs hit 1-31

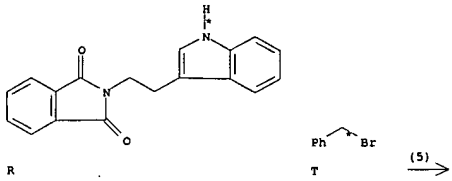
L2 ANSWER 1 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 144:192408 CASREACT
TITLE: Facile Construction of the Pentacyclic Framework of Subincanadine B. Synthesis of 20-Deethylenylated Subincanadine B and 19,20-Dihydrosubincanadine B
AUTHOR(S): Liu, Yanqin; Luo, Shengjun; Fu, Xingnian; Fang, Fang; Zhuang, Zeyang; Xiong, Wanting; Jia, Xueshun; Zhai, Hongbin
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Organic Letters (2006), 8(1), 115-118
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



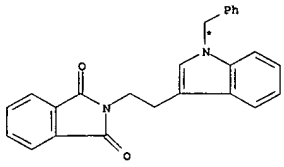
I II

AB We describe a facile approach for effectively constructing the pentacyclic framework of subincanadine B. The seven-step assembly of tetracyclic ketone I featured Michael addition, Pictet-Spengler cyclization, and Dieckmann condensation. From this key ketone intermediate, two analogs of subincanadine B, i.e., 20-deethylenylated subincanadine B (II·Cl-; R = H) and 19,20-dihydrosubincanadine B (II·Cl-; R = Et), were synthesized in four steps, resp.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 68 ...R + T ===> U...



R T



U
YIELD 99%

RX(5)

STAGE(1)
RGT V 7646-69-7 NaH
SOL 68-12-2 DMF
CON room temperature

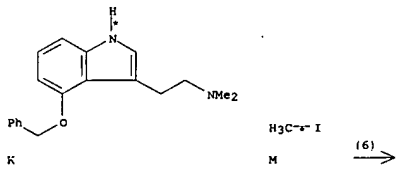
STAGE(2)
RCT R 15741-71-6
SOL 68-12-2 DMF
CON 1 hour, room temperature

STAGE(3)
RCT T 100-39-0
CON overnight, 55 deg C

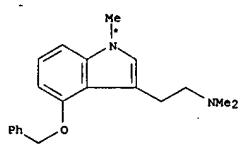
PRO U 874916-37-7

L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:278414 CASREACT
TITLE: SAR of psilocybin analogs: Discovery of a selective 5-HT2C agonist
AUTHOR(S): Sard, Howard; Kumaran, Govindaraj; Morency, Cynthia; Roth, Bryan L.; Toth, Beth Ann; He, Ping; Shuster, Louis
CORPORATE SOURCE: Organix, Inc., Woburn, MA, 01801, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(20), 4555-4559
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An SAR study of psilocybin and psilocin derivs. reveals that 1-methylpsilocin is a selective agonist at the h5-HT2C receptor. The corresponding phosphate derivative, 1-methylpsilocybin, shows efficacy in an animal model for obsessive-compulsive disorder, as does 4-fluoro-N,N-dimethyltryptamine. These results suggest a new area for development of novel 5-HT2C agonists with applications for drug discovery.
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 56 ...K + M ===> N...



K M

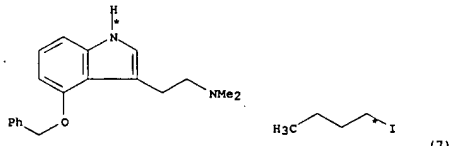


N
YIELD 73%

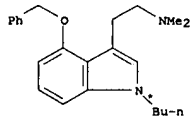
L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(6) RCT K 28383-23-5, M 74-88-4
RGT O 7646-69-7 NaH
PRO N 1640-04-6

RX(7) OF 56 ...K + P ===> Q...



K P

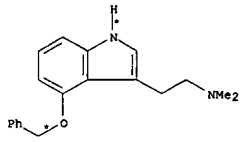


Q
YIELD 48%

RX(7) RCT K 28383-23-5, P 542-69-8
PRO Q 879485-07-1
NTE no experimental detail

RX(33) OF 56 COMPOSED OF RX(6), RX(8)
RX(33) K + M ===> R

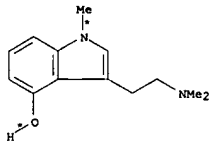
L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



K

M

2 STEPS



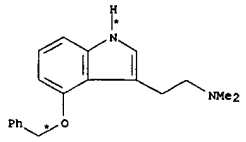
R
YIELD 78%

RX(6) RCT K 28383-23-5, M 74-88-4
RGT O 7646-69-7 NaH
PRO N 1640-04-6

RX(8) RCT N 1640-04-6
RGT S 1333-74-0 H2
PRO R 1465-16-3
CAT 7440-05-3 Pd

RX(34) OF 56 COMPOSED OF RX(7), RX(9)
RX(34) K + P ===> U

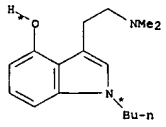
L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



K

P

2 STEPS



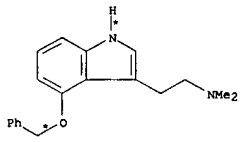
U
YIELD 67%

RX(7) RCT K 28383-23-5, P 542-69-8
PRO Q 879485-07-1
NTE no experimental detail

RX(9) RCT Q 879485-07-1
RGT S 1333-74-0 H2
PRO U 864186-05-0
CAT 7440-05-3 Pd

RX(49) OF 56 COMPOSED OF RX(6), RX(8), RX(10)
RX(49) K + M ===> V

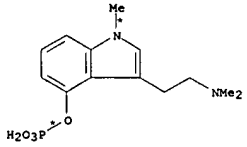
L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



K

M

3 STEPS



V
YIELD 12%

RX(6) RCT K 28383-23-5, M 74-88-4
RGT O 7646-69-7 NaH
PRO N 1640-04-6

RX(8) RCT N 1640-04-6
RGT S 1333-74-0 H2
PRO R 1465-16-3
CAT 7440-05-3 Pd

RX(10) RCT R 1465-16-3

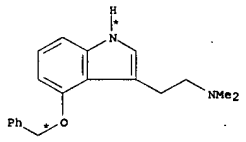
STAGE(1)
RGT W 1623-08-1 (PhCH2O)2P(O)OH, X 4111-54-0 LiN(Pr-i)2

STAGE(2)
RGT S 1333-74-0 H2
CAT 7440-05-3 Pd

PRO V 18483-72-2

RX(51) OF 56 COMPOSED OF RX(7), RX(9), RX(11)
RX(51) K + P ===> Y

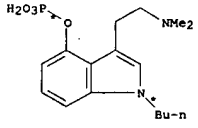
L2 ANSWER 2 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



K

P

3 STEPS



Y
YIELD 26%

RX(7) RCT K 28383-23-5, P 542-69-8
PRO Q 879485-07-1
NTE no experimental detail

RX(9) RCT Q 879485-07-1
RGT S 1333-74-0 H2
PRO U 864186-05-0
CAT 7440-05-3 Pd

RX(11) RCT U 864186-05-0

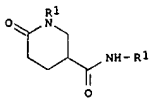
STAGE(1)
RGT W 1623-08-1 (PhCH2O)2P(O)OH, X 4111-54-0 LiN(Pr-i)2

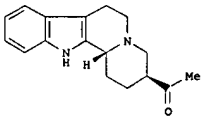
STAGE(2)
RGT S 1333-74-0 H2
CAT 7440-05-3 Pd

PRO Y 864186-06-1

L2 ANSWER 3 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:26761 CASREACT
TITLE: Convenient Synthesis of Substituted Piperidinones from
α,β-Unsaturated Amides: Formal Synthesis of Deplancheine, Tacamonine, and Paroxetine
AUTHOR(S): Takasu, Kiyosei; Nishida, Naoko; Tomimura, Akiko; Ihara, Masataka
CORPORATE SOURCE: Department of Organic Chemistry, Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai, 980-8578, Japan
SOURCE: Journal of Organic Chemistry (2005), 70(10), 3957-3962
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

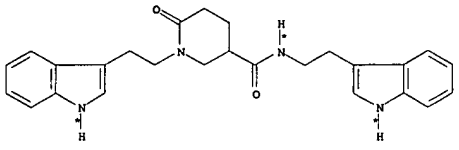

I


II

AB An intermol. aza-double Michael reaction leading to functionalized piperidin-2-ones from simple starting materials has been developed. The method allows α,β-unsatd. amides to be used as a synthon of the piperidine nucleus. For example, reacting H2C:CHCONHR1 (R1 = PhCH2, cyclohexyl, 2-indolylethyl, 2-PhCH2CH2) with TMSI/HDMS or TBSOTf/NEt3 gave the piperidinones I in good to excellent yields. In addition, the utility of this methodol. is demonstrated by its application to a formal synthesis of the indolo[2,3-a]quinolizidine alkaloids, (±)-deplancheine, (±)-tacamonine, and the antidepressant paroxetine. As an illustration, I (R1 = 2-indolylethyl) was converted to (indolo[2,3-a]quinolizidinyl)ethanone II which has previously been transformed into (±)-deplancheine.
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(10) OF 87 ...S + 2 AC ===> AD...

L2 ANSWER 3 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)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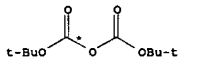
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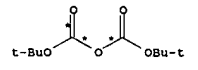
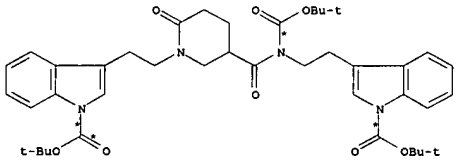

AC

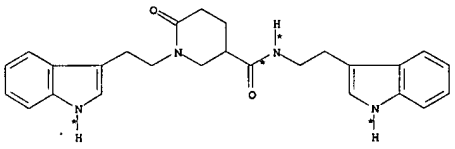
(10)

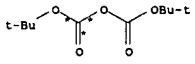

AD
YIELD 96%

RX(10) RCT S 853063-74-8, AC 24424-99-5
RGT I 121-44-8 Et3N
PRO AD 853063-66-8
CAT 1122-58-3 4-DMAP
CON 1 hour, room temperature

RX(39) OF 87 COMPOSED OF RX(10), RX(11)
RX(39) S + 2 AC ===> AF

L2 ANSWER 3 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)


S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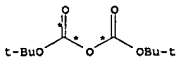
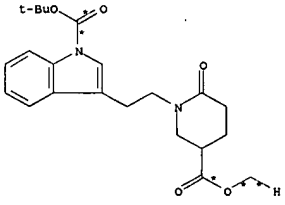

AC

2 STEPS

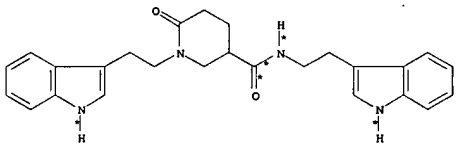

AF
YIELD 86%

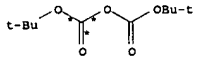
RX(10) RCT S 853063-74-8, AC 24424-99-5
RGT I 121-44-8 Et3N
PRO AD 853063-66-8
CAT 1122-58-3 4-DMAP
CON 1 hour, room temperature

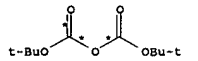
RX(11) RCT AD 853063-66-8
RGT AG 124-41-4 NaOMe
PRO AF 853063-67-9
SOL 67-56-1 MeOH
CON 20 minutes, 0 deg C

L2 ANSWER 3 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

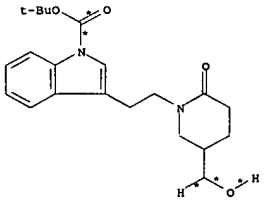
RX(52) OF 87 COMPOSED OF RX(10), RX(11), RX(16)
RX(52) S + 2 AC ===> AV


S


AC


AC

3 STEPS


AV
YIELD 67%

RX(10) RCT S 853063-74-8, AC 24424-99-5
RGT I 121-44-8 Et3N
PRO AD 853063-66-8
CAT 1122-58-3 4-DMAP
CON 1 hour, room temperature

RX(11) RCT AD 853063-66-8
RGT AG 124-41-4 NaOMe
PRO AF 853063-67-9
SOL 67-56-1 MeOH

L2 ANSWER 3 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
CON 20 minutes, 0 deg C

RX(16) RCT AF 853063-67-9

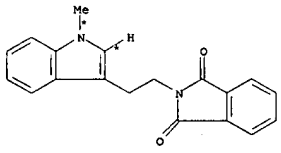
STAGE(1)
RGT AW 16949-15-8 LiBH4, AX 22560-16-3 Superhydride
SOL 109-99-9 THF
CON 6 hours, room temperature

STAGE(2)
RGT AO 7732-18-5 Water

PRO AV 853063-70-4

L2 ANSWER 4 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

3 STEPS



DO
YIELD 97%

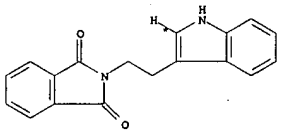
RX(26) RCT BF 15741-71-6
RGT BH 39416-48-3 Pyridinium tribromide
PRO BG 192182-46-0
SOL 109-99-9 THF, 67-66-3 CHCl3
NTE regioselective

RX(35) RCT BG 192182-46-0, BY 98437-24-2
RGT Q 497-19-8 Na2CO3, BN 7447-41-8 LiCl
PRO BZ 849216-93-9
CAT 14221-01-3 Pd(PPh3)4
SOL 64-17-5 EtOH, 108-88-3 PhMe
NTE Suzuki reaction

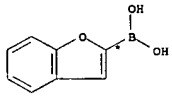
RX(66) RCT BZ 849216-93-9, DN 74-88-4
RGT DP 7646-69-7 NaH
PRO DO 70369-20-9
SOL 68-12-2 DMF

L2 ANSWER 4 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:348129 CASREACT
TITLE: Tryptamine and homotryptamine-based sulfonamides as potent and selective inhibitors of 15-lipoxygenase
AUTHOR(S): Weinstein, David S.; Liu, Wen; Gu, Zhengxiang; Langevine, Charles; Ngu, Khehyong; Fadnis, Leena; Combs, Donald W.; Sitkoff, Doree; Ahmad, Saleem; Zhuang, Shaobin; Chen, Xing; Wang, Feng-Lai; Loughney, Deborah A.; Atwal, Karnail S.; Zahler, Robert; Macor, John E.; Madsen, Cort S.; Murugesan, Natesan
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Bristol-Myers Squibb, Princeton, NJ, 08543, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(5), 1435-1440
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of inhibitors of mammalian 15-lipoxygenase based on tryptamine and homotryptamine scaffolds is described. Compds. with aryl substituents at C-2 of the indole core of tryptamine and homotryptamine sulfonamides proved to be potent inhibitors of the isolated enzyme. Selected compds. also demonstrated desirable inhibition selectivities over isoenzymes 5- and P-12-LO.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(142) OF 196 COMPOSED OF RX(26), RX(35), RX(66)
RX(142) BF + BY + DN ===> DO



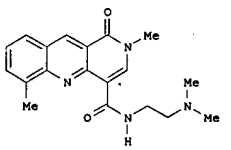
BF



BY

DN

L2 ANSWER 5 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:298020 CASREACT
TITLE: Synthesis and cytotoxic activity of carboxamide derivatives of benzo[b][1,6]naphthyridin-(5H)ones
AUTHOR(S): Deady, Leslie W.; Rogers, Michael L.; Zhuang, Li; Baguley, Bruce C.; Denny, William A.
CORPORATE SOURCE: Chemistry Department, La Trobe University, 3086, Australia
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(4), 1341-1355
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

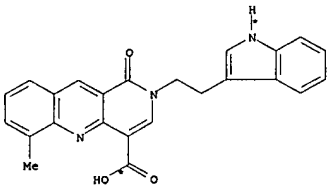


I

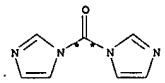
AB A previous reaction leading to 2-substituted 6-methyl-1-oxo-1,2-dihydrobenzo[b][1,6]naphthyridine-4-carboxylic acids has been extended to encompass a broad range of 2-substituents. Carboxamides, e.g., I, particularly 4-N-(2-(dimethylamino)ethyl], were tested for growth inhibitory properties. Potent cytotoxicity against murine P388 leukemia and Lewis lung carcinoma (LLTC) was retained for compds. bearing a remarkably diverse range of 2-substituents with a number having IC50 values <10 nM. Five of the compds. were tested in vivo against s.c. colon 38 tumors in mice; a single dose (1.8 mg/kg) proved curative for the 2-(4-fluorophenyl) derivative, a further increase in potency over the very effective 2-Me analog reported previously.
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(56) OF 186 ...AQ + BQ + 2 BO ===> CB...

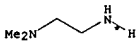
L2 ANSWER 5 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AQ

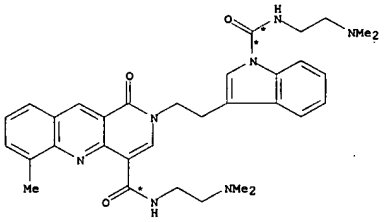


BQ



2 BQ

(56)



CB
YIELD 62%

RX(56) RCT AQ 627093-64-5, BQ 530-62-1

STAGE(1)
SOL 123-91-1 Dioxane
CON 48 hours, reflux

L2 ANSWER 5 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)
RCT BO 108-00-9
SOL 75-09-2 CH2Cl2
CON 16 hours, room temperature

PRO CB 627093-92-9

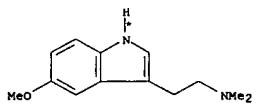
L2 ANSWER 6 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:424159 CASREACT
TITLE: Novel 5-HT7 Receptor Inverse Agonists. Synthesis and Molecular Modeling of Arylpiperazine- and 1,2,3,4-Tetrahydroisoquinoline-Based Arylsulfonamides
AUTHOR(S): Vermeulen, Erik S.; Van Smeden, Marjan; Schmidt, Anne W.; Sprouse, Jeffrey S.; Wikstroem, Haakan V.; Grol, Cor J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Center for Pharmacy, State University of Groningen, Groningen, NL-9713, Neth.
SOURCE: Journal of Medicinal Chemistry (2004), 47(22), 5451-5466
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

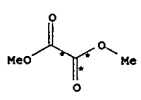
AB A series of arylpiperazine- and 1,2,3,4-tetrahydroisoquinoline-based arylsulfonamides was synthesized and evaluated for their interactions with the constitutively active 5-HT7 receptor. Effects on basal adenylate cyclase activity were measured using HEK-293 cells expressing the rat 5-HT7. All ligands produced a decrease of adenylate cyclase activity, indicative of their inverse agonism. Addnl., computational studies with a set of 22 inverse agonists, including these novel inverse agonists and inverse agonists known from literature, resulted in a pharmacophore model and a CoMFA model (R2 = 0.97, SE = 0.18). Docking of inverse agonists at the binding site of a model of the helical parts of the 5-HT7 receptor, based on the α carbon template for 7-TM GPCRs, revealed interesting mol. interactions and a possible explanation for observed structure-activity relationships.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(26) OF 111 ...AY + BA ===> BB



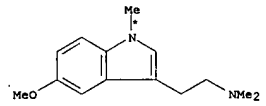
AY



BA

(26)

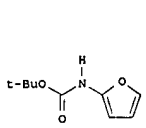
L2 ANSWER 6 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

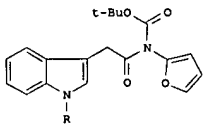


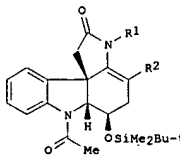
BB
YIELD 86%

RX(26) RCT AY 1019-45-0, BA 553-90-2
RGT BC 865-47-4 t-BuOK
PRO BB 103858-17-9
SOL 68-12-2 DMF
CON 4 hours, reflux

L2 ANSWER 7 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:38763 CASREACT
TITLE: A New Strategy toward Indole Alkaloids Involving an Intramolecular Cycloaddition/Rearrangement Cascade
AUTHOR(S): Padwa, Albert; Brodney, Michael A.; Lynch, Stephen M.; Rashatasakhon, Paitoon; Wang, Qiu; Zhang, Hongjun
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Journal of Organic Chemistry (2004), 69(11), 3735-3745
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

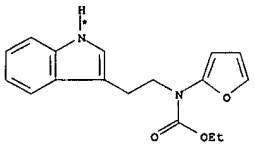

I


II


III

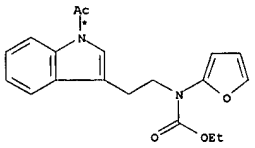
AB The intramol. Diels-Alder reaction between an amidofuran moiety tethered onto an indole component was examined as a strategy for the synthesis of Aspidosperma alkaloids. Furanyl carbamate I was acylated using a mixed anhydride of indole acetic acid to provide amidofuran II (R = H) in 68% yield. Further N-acylation of this indole furnished II (R = C(O)Me) in 88% yield. Cyclization precursors were prepared by removing the carbamate moiety followed by N-alkylation with the appropriate alkyl halides. Large substituent groups on the amido nitrogen atom causes the reactive s-trans conformation of the amidofuran to be more highly populated, thereby facilitating the Diels-Alder cycloaddn. The reaction requires the presence of an electron-withdrawing substituent on the indole nitrogen in order for the cycloaddn. to proceed. Treatment of N-allyl-bromoenamide III (R1 = allyl, R2 = Br) with n-Bu3SnH/AIBN preferentially led to the 6-endo trig cyclization product III (R1, R2 = (CH2)3), with the best yield (91%) being obtained under high diln. conditions. The initially generated cyclohexenyl radical derived from III (R1 = allyl, R2 = Br) produces the pentacyclic heterocycle III (R1, R2 = (CH2)3) by either a direct 6-endo trig cyclization or, alternatively, by a vinyl radical rearrangement pathway.
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 206 ...H + L ===> M...


H


L

(3)


M

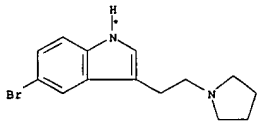
YIELD 90%

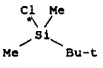
RX(3) RCT H 212561-12-1
STAGE(1)

L2 ANSWER 7 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
RGT N 32503-27-8 Bu4N.HSO4, O 1310-73-2 NaOH
SOL 75-09-2 CH2Cl2
CON 5 minutes, room temperature
STAGE(2)
RCT L 75-36-5
CON 1 hour, room temperature
STAGE(3)
RGT F 7732-18-5 Water
PRO M 212561-13-2

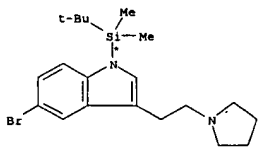
L2 ANSWER 8 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 140:287242 CASREACT
TITLE: 3-(2-Pyrrolidin-1-ylethyl)-5-(1,2,3,6-tetrahydropyridin-4-yl)-1H-indole derivatives as high affinity human 5-HT1b/1D ligands
AUTHOR(S): Egle, Ian; MacLean, Neil; Demchyshyn, Lidia; Edwards, Louise; Slassi, Abdelmalik; Tehim, Ashok
CORPORATE SOURCE: NPS Pharmaceuticals Inc, Mississauga, ON, 6850, Can.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(3), 727-729
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 3-(2-pyrrolidin-1-ylethyl)-5-(1,2,3,6-tetrahydropyridin-4-yl)-1H-indole derivs. has been prepared using parallel synthesis techniques, and their structure-activity relationships studied. High affinity human 5-HT1b/1D (h5-HT1b/1D) ligands have been identified.
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 129 ...G + J ===> K...


G


J

(3)

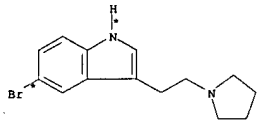

K

RX(3) RCT G 17274-68-9, J 18162-48-6

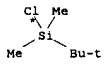
L2 ANSWER 8 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT L 1070-89-9 (Me3Si)2N.Na
PRO K 255711-67-2
SOL 68-12-2 DMF
CON 0 deg C

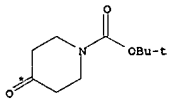
RX(27) OF 129 COMPOSED OF RX(3), RX(4)
RX(27) G + J + M ===> N



G

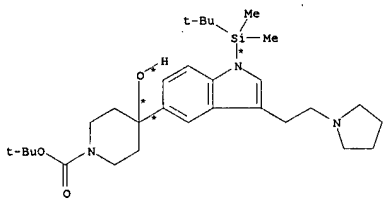


J



M

2 STEPS



N
YIELD 48%

L2 ANSWER 8 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(3) RCT G 17274-68-9, J 18162-48-6
RGT L 1070-89-9 (Me3Si)2N.Na
PRO K 255711-67-2
SOL 68-12-2 DMF
CON 0 deg C

G, J

RX(4) RCT K 255711-67-2

STAGE(1)
RGT O 594-19-4 t-BuLi
SOL 109-99-9 THF, 109-66-0 Pentane
CON 1 hour, -78 deg C

STAGE(2)
RCT M 79099-07-3
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C -> room temperature
SUBSTAGE(2) 2 hours, room temperature

M

STAGE(3)
RGT P 12408-02-5 H+
CON pH 7

PRO N 675841-44-8

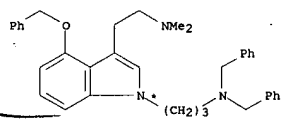
Silyl

only silyl rxn (bad date)

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 138:205240 CASREACT
TITLE: Synthesis of a psilocin hapten and a protein-hapten conjugate
AUTHOR(S): Albers, Christian; Lehr, Matthias; Beike, Justus; Kohler, Helga; Brinkmann, Bernd
CORPORATE SOURCE: Institute of Pharmaceutical and Medicinal Chemistry, University of Munster, Munster, D-48149, Germany
SOURCE: Journal of Pharmacy and Pharmacology (2002), 54(9), 1265-1270
CODEN: JPPMAB; ISSN: 0022-3573
PUBLISHER: Pharmaceutical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Derivs. of psilocin with ω-functionalized alkyl spacers in position 1 of the indole ring were synthesized as haptens for use in a RIA. Whereas the psilocin analogs with a 3-aminopropyl and a 4-aminobutyl moiety at the indole nitrogen decomposed during synthesis, the analogous 3-carboxypropyl psilocin derivative proved to be stable. This compound was coupled to bovine serum albumin (BSA) using the N-hydroxysuccinimide ester-mediated conjugation. The protein-hapten conjugate was characterized by matrix-assisted laser desorption ionization mass spectrometry. The mass spectrometry data indicated an average incorporation ratio of 4-5 mols. of psilocin hapten per mol. of BSA.
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Sept 2002

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



C
YIELD 74%

R2 = sub. alkyl

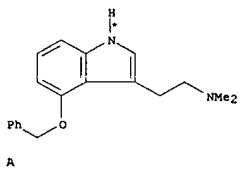
RX(1) RCT A 28383-23-5

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

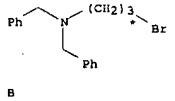
STAGE(2)
RCT B 98346-35-1
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 4 hours, 60 deg C
SUBSTAGE(3) overnight, room temperature

PRO C 500003-01-0

RX(1) OF 9 A + B ===> C



A

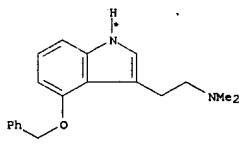


B

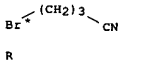
(1)

R1 = sub alkoxy ✓

RX(5) OF 9 A + R ===> F...



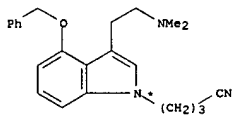
A



R

(5)

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



F
YIELD 49%

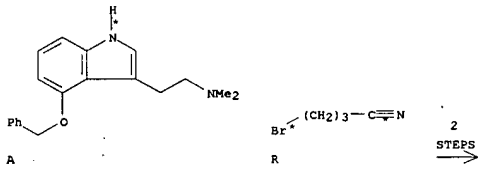
RX(5) RCT A 28383-23-5

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

STAGE(2)
RCT R 5332-06-9
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) overnight, room temperature

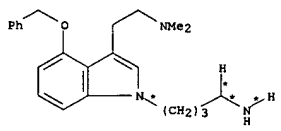
PRO F 500003-02-1

RX(7) OF 9 COMPOSED OF RX(5), RX(2)
RX(7) A + R ===> G



A R

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



G
YIELD 86%

RX(5) RCT A 28383-23-5

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

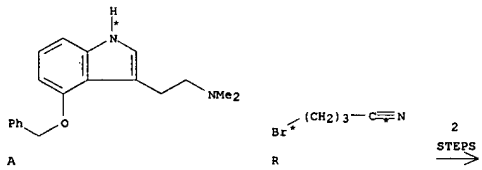
STAGE(2)
RCT R 5332-06-9
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) overnight, room temperature

PRO F 500003-02-1

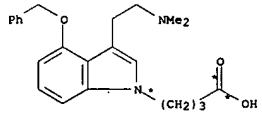
RX(2) RCT F 500003-02-1
RGT H 1333-74-0 H2
PRO G 500003-03-2
CAT 7440-02-0 Ni
SOL 67-56-1 MeOH
CON 38 hours, room temperature
NTE Raney nickel used

RX(8) OF 9 COMPOSED OF RX(5), RX(3)
RX(8) A + R ===> K

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



A R



K
YIELD 36%

RX(5) RCT A 28383-23-5

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

STAGE(2)
RCT R 5332-06-9
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) overnight, room temperature

PRO F 500003-02-1

RX(3) RCT F 500003-02-1

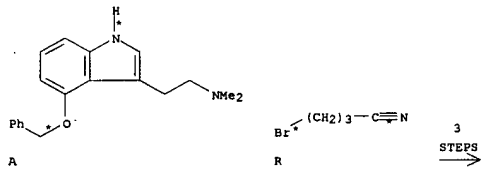
STAGE(1)
RGT L 1310-58-3 KOH
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 10 hours, reflux

STAGE(2)
RGT M 7647-01-0 HCl
SOL 7732-18-5 Water

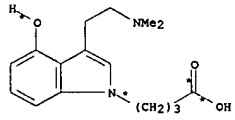
PRO K 500003-04-3

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(9) OF 9 COMPOSED OF RX(5), RX(3), RX(4)
RX(9) A + R ===> P



A R



P
YIELD 95%

RX(5) RCT A 28383-23-5

STAGE(1)
RGT D 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

STAGE(2)
RCT R 5332-06-9
SOL 68-12-2 DMF
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) overnight, room temperature

PRO F 500003-02-1

RX(3) RCT F 500003-02-1

STAGE(1)
RGT L 1310-58-3 KOH
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 10 hours, reflux

STAGE(2)

L2 ANSWER 9 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

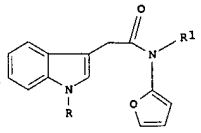
RGT M 7647-01-0 HCl
SOL 7732-18-5 Water

PRO K 500003-04-3

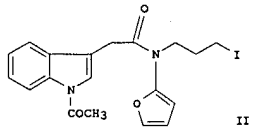
RX(4) RCT K 500003-04-3
RGT H 1333-74-0 H2
PRO P 500003-05-4
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 2 hours, room temperature

L2 ANSWER 10 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

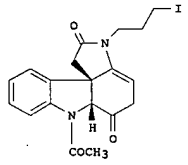
ACCESSION NUMBER: 138:137448 CASREACT
TITLE: Intramolecular Amidofuran Cycloadditions across an Indole π-Bond: An Efficient Approach to the Aspidosperma and Strychnos ABCE Core
AUTHOR(S): Lynch, Stephen M.; Bur, Scott K.; Padwa, Albert
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2002), 4(26), 4643-4645
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II



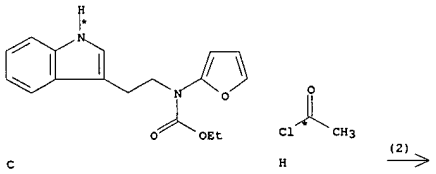
III

AB The intramol. Diels-Alder reaction between an amidofuran moiety tethered onto an indole component was examined as a strategy for the synthesis of Aspidosperma and Strychnos alkaloids. Furanyl carbamate was acylated using a mixed anhydride to provide amidofuran I (R = H, R1 = CO2CMe3) in 68% yield. Further N-acylation of this indole furnished I (R = COMe, R1 = CO2CMe3) in 88% yield. Cyclization precursors were prepared by removing the carbamate moiety followed by N-alkylation with the appropriate alkyl halides. Thermolysis of II provided the novel tetracyclic ketone III in 74% yield.

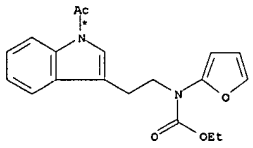
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 10 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(2) OF 59 ...C + H ===> I...



C H (2) →



I
YIELD 90%

RX(2) RCT C 212561-12-1

STAGE(1)
RGT J 32503-27-8 Bu4N.HSO4, K 1310-73-2 NaOH
SOL 75-09-2 CH2Cl2
CON 5 minutes, room temperature

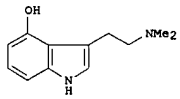
STAGE(2)
RCT H 75-36-5
CON 1 hour, room temperature

STAGE(3)
RGT E' 7732-18-5 Water
CON room temperature

PRO I 212561-13-2

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:263284 CASREACT
TITLE: The chemistry of indoles. Part 109. Synthetic studies of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position
AUTHOR(S): Yamada, Fumio; Tamura, Mayumi; Hasegawa, Atsuko; Somei, Masanori
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1), 92-99
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

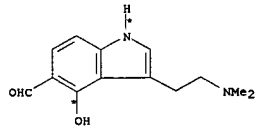


I

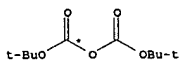
AB Psilocin (I) analogs having either a formyl group or a bromine atom at the 5- or 7-position have been prepared for the first time. Syntheses of 5- and 7-bromo derivs. of 4-hydroxy- and 4-benzyloxyindole-3-carbaldehyde, 4-benzyloxyindole-3-acetonitriles, and 4-benzyloxy-N,N-dimethyltryptamine have also been established.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 114 ...C + I ===> J

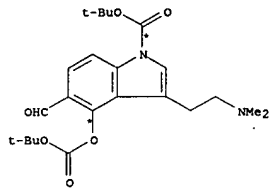


C



I (3) →

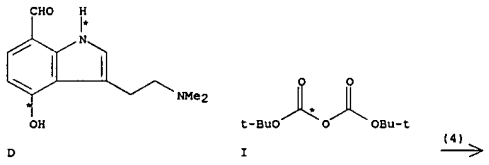
L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



J
YIELD 78%

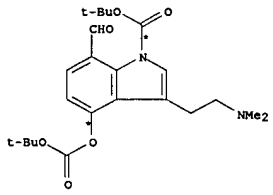
RX(3) RCT C 404887-81-6, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO J 404887-84-9
SOL 75-09-2 CH2Cl2

RX(4) OF 114 ...D + I ===> M



D I (4)

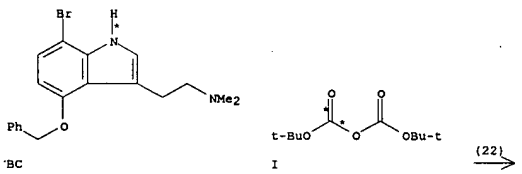
L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



M
YIELD 66%

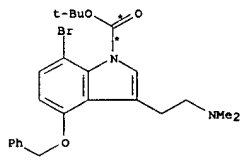
RX(4) RCT D 404887-83-8, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO M 404887-85-0
SOL 75-09-2 CH2Cl2

RX(22) OF 114 ...BC + I ===> BH



BC I (22)

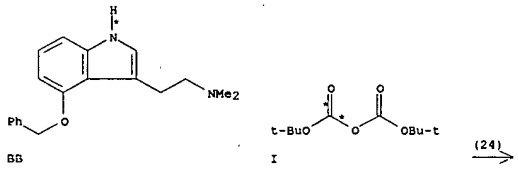
L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



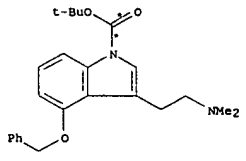
BH
YIELD 83%

RX(22) RCT BC 404888-06-8, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BH 404888-08-0
SOL 75-09-2 CH2Cl2

RX(24) OF 114 BB + I ===> BL...



BB I (24)

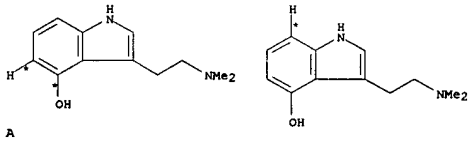


BL
YIELD 96%

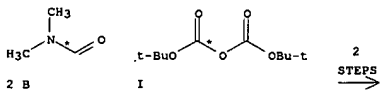
L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(24) RCT BB 28383-23-5, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BL 404888-10-4
SOL 75-09-2 CH2Cl2

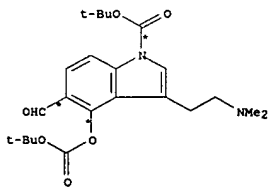
RX(31) OF 114 COMPOSED OF RX(1), RX(3)
RX(31) 2 A + 2 B + I ===> J



A A



2 B I 2 STEPS



J
YIELD 78%

RX(1) RCT A 520-53-6, B 68-12-2

STAGE(1)
RGT E 10025-87-3 POCl3
SOL 68-12-2 DMF

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

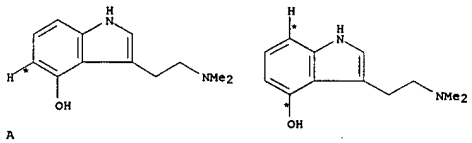
STAGE(2)
RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water

STAGE(3)
RGT G 7647-01-0 HCl
SOL 7732-18-5 Water

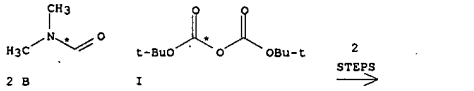
PRO C 404887-81-6, D 404887-83-8
NTE yield depends on reaction conditions

RX(3) RCT C 404887-81-6, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO J 404887-84-9
SOL 75-09-2 CH2Cl2

RX(32) OF 114 COMPOSED OF RX(1), RX(4)
RX(32) 2 A + 2 B + I ===> M



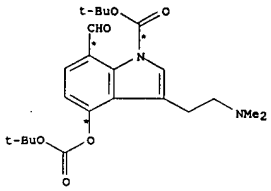
A A



2 B I

2 STEPS

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



M
YIELD 66%

RX(1) RCT A 520-53-6, B 68-12-2

STAGE(1)
RGT E 10025-87-3 POCl3
SOL 68-12-2 DMF

STAGE(2)
RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water

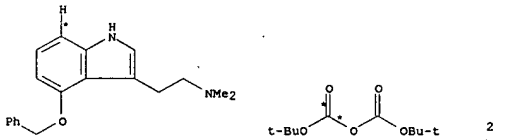
STAGE(3)
RGT G 7647-01-0 HCl
SOL 7732-18-5 Water

PRO C 404887-81-6, D 404887-83-8
NTE yield depends on reaction conditions

RX(4) RCT D 404887-83-8, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO M 404887-85-0
SOL 75-09-2 CH2Cl2

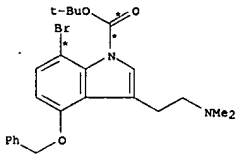
RX(47) OF 114 COMPOSED OF RX(20), RX(22)
RX(47) BB + I ===> BH

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BB I

2 STEPS



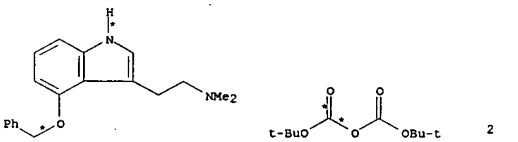
BH
YIELD 83%

RX(20) RCT BB 28383-23-5
RGT W 110-86-1 Pyridine, X 10035-10-6 HBr, Y 7726-95-6 Br2
PRO BC 404888-06-8
SOL 67-66-3 CHCl3, 60-29-7 Et2O

RX(22) RCT BC 404888-06-8, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BH 404888-08-0
SOL 75-09-2 CH2Cl2

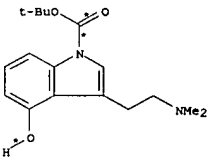
RX(52) OF 114 COMPOSED OF RX(24), RX(25)
RX(52) BB + I ===> BM

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BB I

2 STEPS



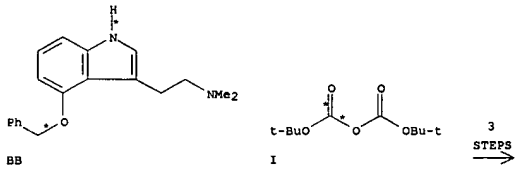
BM
YIELD 93%

RX(24) RCT BB 28383-23-5, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BL 404888-10-4
SOL 75-09-2 CH2Cl2

RX(25) RCT BL 404888-10-4
RGT AK 1333-74-0 H2
PRO BM 404888-11-5
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

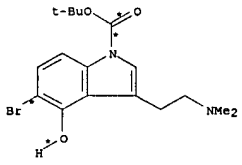
RX(81) OF 114 COMPOSED OF RX(24), RX(25), RX(26)
RX(81) BB + I ===> BI

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BB I

3 STEPS



BI
YIELD 87%

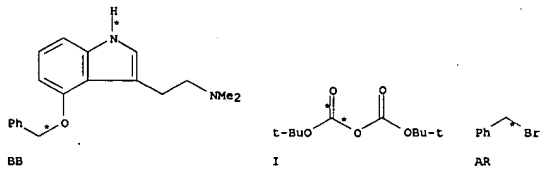
RX(24) RCT BB 28383-23-5, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BL 404888-10-4
SOL 75-09-2 CH2Cl2

RX(25) RCT BL 404888-10-4
RGT AK 1333-74-0 H2
PRO BM 404888-11-5
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

RX(26) RCT BM 404888-11-5
RGT W 110-86-1 Pyridine, X 10035-10-6 HBr, Y 7726-95-6 Br2
PRO BI 404888-12-6
SOL 67-66-3 CHCl3, 60-29-7 Et2O

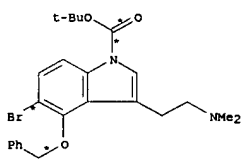
RX(84) OF 114 COMPOSED OF RX(24), RX(25), RX(26), RX(23)
RX(84) BB + I + AR ===> BJ

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BB I AR

4 STEPS



BJ
YIELD 43%

RX(24) RCT BB 28383-23-5, I 24424-99-5
RGT K 1122-58-3 4-DMAP
PRO BL 404888-10-4
SOL 75-09-2 CH2Cl2

RX(25) RCT BL 404888-10-4
RGT AK 1333-74-0 H2
PRO BM 404888-11-5
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

RX(26) RCT BM 404888-11-5
RGT W 110-86-1 Pyridine, X 10035-10-6 HBr, Y 7726-95-6 Br2
PRO BI 404888-12-6
SOL 67-66-3 CHCl3, 60-29-7 Et2O

L2 ANSWER 11 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(23) RCT BI 404888-12-6

STAGE(1)
RGT BK 7693-26-7 KH
SOL 68-12-2 DMF

STAGE(2)
RCT AR 100-39-0
SOL 68-12-2 DMF

STAGE(3)
SOL 7732-18-5 Water

PRO BJ 404888-09-1

L2 ANSWER 12 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

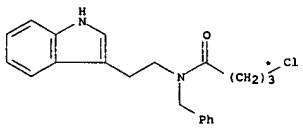
ACCESSION NUMBER: 135:371593 CASREACT
TITLE: New bis-indolic macrolactams
AUTHOR(S): Henin, Jacques; Noe, Eric; Laronze, Jean-Yves
CORPORATE SOURCE: Laboratoire de Chimie Therapeutique, UMR-CNRS 6013, IFR no 53 Biomolecules, UFR de Pharmacie, Reims, 51096, Fr.
SOURCE: Synthesis (2001), (11), 1693-1703
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Treatment of several ω-halogenoamides, e.g. I, derived from tryptamine, with powdered potassium hydroxide in 1,2-dimethoxyethane in the presence of 18-crown-6, resulted in intramol. and/or bimol. cyclization, depending on the length of the chain and dilution conditions, to give macrocyclic compds, e.g. II and III. Some of them were converted by a Bischler-Napieralski reaction, followed by sodium borohydride reduction, to new tetracyclic derivs. of β-carbolines, e.g. IV.

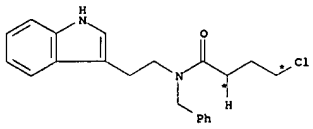
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 36 ...3 G ===> O + P

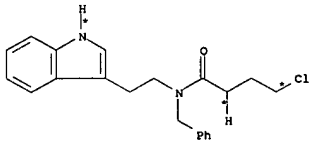


G

L2 ANSWER 12 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

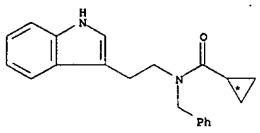


G



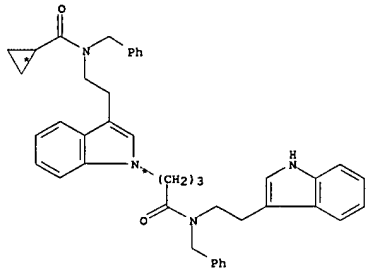
G

(6)



O
YIELD 36%

L2 ANSWER 12 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



P
YIELD 7%

RX(6) RCT G 374558-11-9
RGT J 1310-58-3 KOH, K 17455-13-9 18-Crown-6
PRO O 292029-81-3, P 374558-17-5
SOL 110-71-4 (CH2OMe)2
NTE in the dark

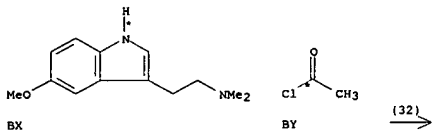
L2 ANSWER 13 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:222891 CASREACT
TITLE: The chemistry of indoles. CIII. Simple syntheses of serotonin, N-methylserotonin, bufotenine, 5-methoxy-N-methyltryptamine, bufobutanoic acid, N-(indol-3-yl)methyl-5-methoxy-N-methyltryptamine, and lespedamine based on 1-hydroxyindole chemistry
AUTHOR(S): Somei, Masanori; Yamada, Fumio; Kurauchi, Takashi; Nagahama, Yoshiyuki; Hasegawa, Masakazu; Yamada, Koji; Teranishi, Sakiko; Sato, Haruhiko; Kaneko, Chikara
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(1), 87-96
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Application of regioselective nucleophilic substitution reactions of 1-hydroxytryptamines to novel and simple syntheses of serotonin, N-methylserotonin, bufotenine, 5-methoxy-N-methyltryptamine, bufobutanoic acid, N-(indol-3-yl)methyl-5-methoxy-N-methyltryptamine, and lespedamine are described. Effective syntheses of 5-benzyloxytryptamine and 1-methoxy-2-oxindoles are also reported.

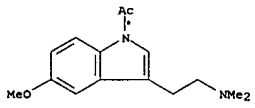
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(32) OF 146 BX + BY ===> BZ



BX BY

(32)



BZ
YIELD 50%

RX(32) RCT BX 1019-45-0

L2 ANSWER 13 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(1)
RGT BM 7646-69-7 NaH
SOL 68-12-2 DMF

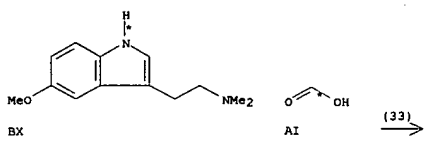
STAGE(2)
RCT BY 75-36-5
SOL 68-12-2 DMF

STAGE(3)
RGT U 1310-73-2 NaOH

STAGE(4)
SOL 67-66-3 CHCl3, 67-56-1 MeOH

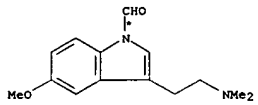
PRO BZ 39998-63-5

RX(33) OF 146 BX + AI ===> CA



BX AI

(33)



CA
YIELD 32%

RX(33) RCT BX 1019-45-0, AI 64-18-6
PRO CA 329763-96-4
SOL 64-18-6 HCO2H

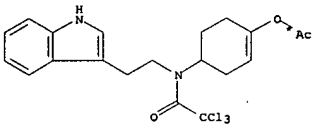
L2 ANSWER 14 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 131:102170 CASREACT
TITLE: Radical promoted cyclizations of trichloroacetamides with silyl enol ethers and enol acetates: the role of the hydride reagent [tris(trimethylsilyl)silane vs. tributylstannane]
AUTHOR(S): Quirante, Josefina; Escolano, Carmen; Diaba, Faiza; Bonjoch, Josep
CORPORATE SOURCE: Faculty of Pharmacy, Laboratory of Organic Chemistry, University of Barcelona, Barcelona, 08028, Spain
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (9), 1157-1162
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reactions between 1-(carbamoyl)dichloromethyl radicals and electron-rich alkenes acting as radical acceptors are reported for the first time. The intramol. reaction of trichloroacetamides with silyl enol ethers gives ketones using (TMS)3SiH as the mediator, alcs. when using Bu3SnH. The reaction with enol acetates gives acetates using either of the above hydride reagents. These radical processes have been applied to the synthesis of 2-azabicyclo[3.3.1]nonanes.

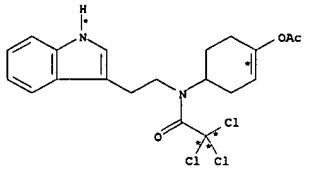
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(12) OF 20 ...2 AA ===> AC



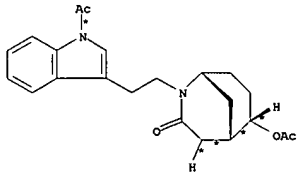
AA

L2 ANSWER 14 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AA

(12)



AC
YIELD 60%

RX(12) RCT AA 230951-61-8

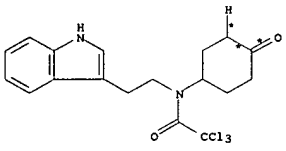
STAGE(1)
RGT N 78-67-1 AIBN
SOL 71-43-2 Benzene

STAGE(2)
RGT O 1873-77-4 (Me3Si)3SiH

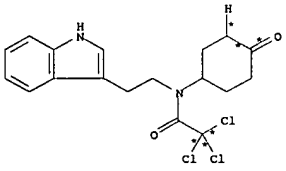
PRO AC 230951-62-9

RX(20) OF 20 COMPOSED OF RX(10), RX(12)
RX(20) 2 Y + 2 I ===> AC

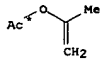
L2 ANSWER 14 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Y

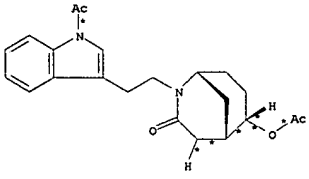


Y



2 I

2 STEPS



AC
YIELD 60%

RX(10) RCT Y 171367-15-0, I 108-22-5

STAGE(1)
RGT K 104-15-4 TsOH
SOL 108-22-5 H2C:CMeOAc

L2 ANSWER 14 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)
RGT E 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO AA 230951-61-8

RX(12) RCT AA 230951-61-8

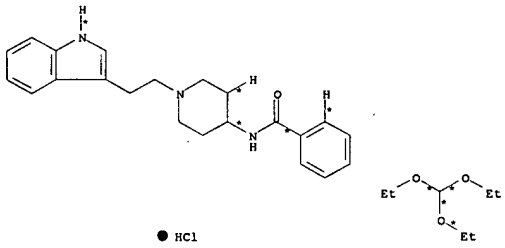
STAGE(1)
RGT N 78-67-1 AIBN
SOL 71-43-2 Benzene

STAGE(2)
RGT O 1873-77-4 (Me3Si)3SiH

PRO AC 230951-62-9

L2 ANSWER 15 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 113:171965 CASREACT
TITLE: First electrophilic substitution of (-)-agroclavine, indoramine, phenothiazine, chlorpromazine, iminodibenzyl, imipramine, and phenazone with triethyl orthoformate as an al-synthon
AUTHOR(S): Pindur, Ulf; Witzel, Helmut
CORPORATE SOURCE: Inst. Pharm., Univ. Mainz, Mainz, D-6500/1, Germany
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1990), 323(7), 439-42
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Agroclavine, imipramine, hydrochloride, and phenazone reacted with tri-Et orthoformate under acid catalysis in an electrophilic, tandem substitution reaction to furnish C3-sym. tris(heteroaryl)methanes while indoramine, phenothiazine, and iminodibenzyl were formylated, ethylated, or ethoxymethylated.. The ambident electrophilic reactivity of tri-Et orthoformate as an al-synthon was clearly apparent.

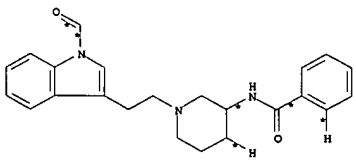
RX(7) OF 7 T + B ===> U



T B

(7)

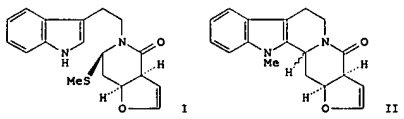
L2 ANSWER 15 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



U
YIELD 44%

RX(7) RCT T 38821-52-2, B 122-51-0
RGT D 76-03-9 Cl3CCO2H
PRO U 129961-35-9
SOL 122-51-0 CH(OEt)3
NTE 40% E-rotamer, 60% Z-rotamer

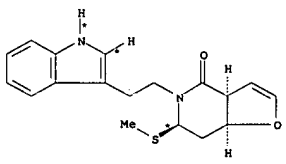
L2 ANSWER 16 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 112:98939 CASREACT
TITLE: Intramolecular cyclization of (methylthio)furopyridones
AUTHOR(S): Naito, Takeaki; Miyata, Okiko; Ninomiya, Ichiya
CORPORATE SOURCE: Kobe Women's Coll. Pharm., Kobe, 658, Japan
SOURCE: Heterocycles (1989), 29(3), 459-62
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

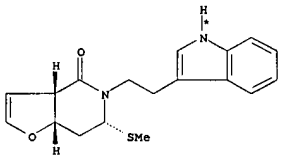
AB Methylthiofuropyridone I is potential synthon for the construction of indoloquinolizidine derivs., e.g. II, by the intramol. cyclization involving methylthio and lactam carbonyl groups.

RX(4) OF 50 ...3 G ===> J + K + L



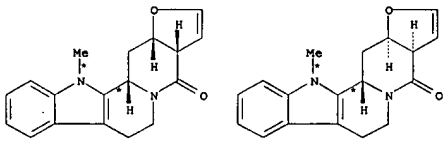
2 G

L2 ANSWER 16 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

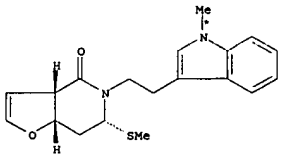


G

(4)



J K
YIELD 24% YIELD 24%

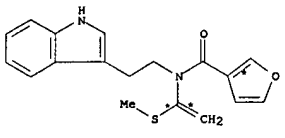


L
YIELD 21%

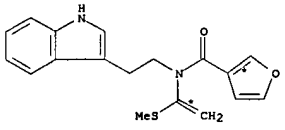
RX(4) RCT G 125218-02-2
RGT M 584-08-7 K2CO3, N 74-88-4 MeI
PRO J 125218-06-6, K 125279-28-9, L 125218-03-3

RX(14) OF 50 COMPOSED OF RX(3), RX(4)
RX(14) 4 F ===> J + K + L

L2 ANSWER 16 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

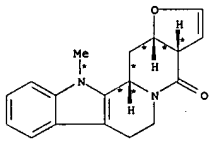


2 F

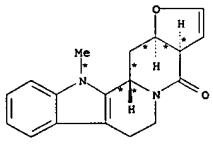


2 F

2 STEPS

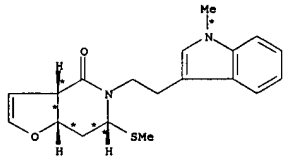


J
YIELD 24%



K
YIELD 24%

L2 ANSWER 16 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



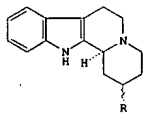
L
YIELD 21%

RX(3) RCT F 125218-01-1
RGT I 16940-66-2 NaBH4
PRO G 125218-02-2, H 125279-27-8
NTE photochem.

RX(4) RCT G 125218-02-2
RGT M 584-08-7 K2CO3, N 74-88-4 MeI
PRO J 125218-06-6, K 125279-28-9, L 125218-03-3

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

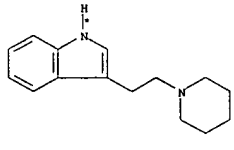
ACCESSION NUMBER: 112:98416 CASREACT
TITLE: Stereoregulation of the C(12b)H-C(2)H relationship in the preparation of 2-substituted 1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinolizines
AUTHOR(S): Lounasmaa, Mauri; Jokela, Reija
CORPORATE SOURCE: Lab. Org. Bioorg. Chem., Tech. Univ. Helsinki, Espoo, SF-02150, Finland
SOURCE: Tetrahedron (1989), 45(12), 3975-92
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



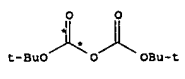
R I

AB Stereochem. control in the preparation of 2-substituted 1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinolizines I (R = H, Me, CMe3), possessing at will the C(12b)H-C(2)H cis- or trans-configuration was achieved by catalytic reduction of the 2,3-dehydro analogs, which were either unsubstituted on the indole nitrogen or substituted with Me3CCO group, resp. The contribution of different conformations to the conformational equilibrium of the prepared compds. was estimated by 13C NMR spectral anal.

RX(29) OF 137 ...AQ + Z ===> AT...



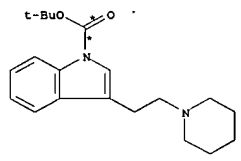
AQ



Z

(29)

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AT
YIELD 90%

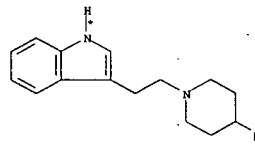
RX(29) RCT AQ 26628-87-5

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

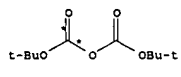
STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AT 125260-53-9

RX(30) OF 137 ...AR + Z ===> AU...



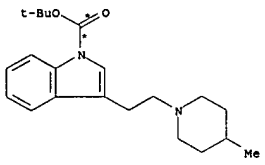
AR



Z

(30)

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AU
YIELD 85%

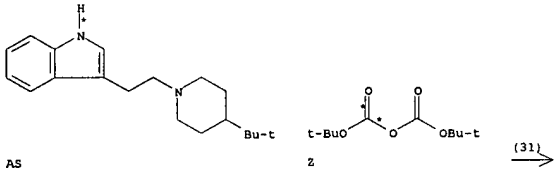
RX(30) RCT AR 125260-52-8

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

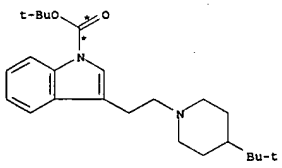
PRO AU 125260-54-0

RX(31) OF 137 ...AS + Z ===> AV...



AS Z

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AV
YIELD 85%

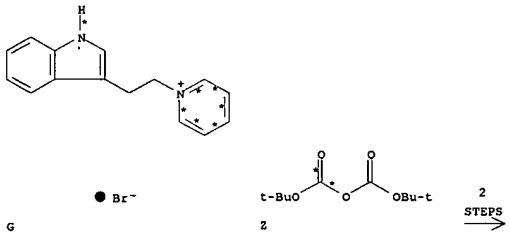
RX(31) RCT AS 58534-26-2

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

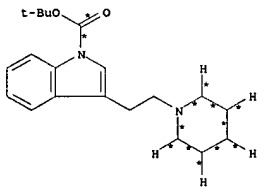
PRO AV 125260-55-1

RX(62) OF 137 COMPOSED OF RX(26), RX(29)
RX(62) G + Z ===> AT



G Z

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AT
YIELD 90%

RX(26) RCT G 50676-26-1
RGT V 1333-74-0 H2
PRO AQ 26628-87-5
CAT 1314-15-4 PtO2

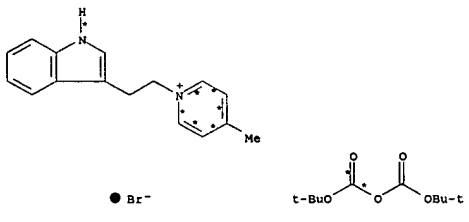
RX(29) RCT AQ 26628-87-5

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

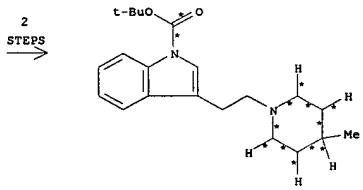
PRO AT 125260-53-9

RX(63) OF 137 COMPOSED OF RX(27), RX(30)
RX(63) C + Z ===> AU



C Z

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AU
YIELD 85%

RX(27) RCT C 24716-26-5
RGT V 1333-74-0 H2
PRO AR 125260-52-8
CAT 1314-15-4 PtO2

RX(30) RCT AR 125260-52-8

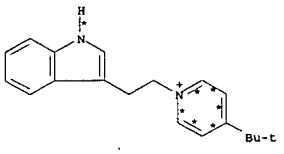
STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

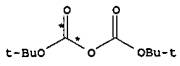
PRO AU 125260-54-0

RX(64) OF 137 COMPOSED OF RX(28), RX(31)
RX(64) E + Z ===> AV

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

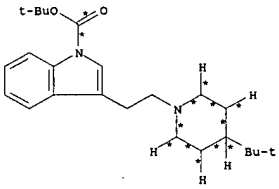


E



Z

2 STEPS



AV
YIELD 85%

RX(28) RCT E 125285-65-6
RGT V 1333-74-0 H2
PRO AS 58534-26-2
CAT 1314-15-4 PtO2

RX(31) RCT AS 58534-26-2

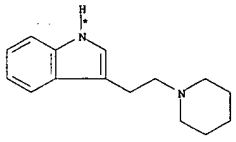
STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

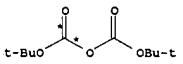
L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO AV 125260-55-1

RX(65) OF 137 COMPOSED OF RX(29), RX(32)
RX(65) AQ + Z ===> AW

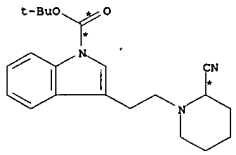


AQ



Z

2 STEPS



AW
YIELD 55%

RX(29) RCT AQ 26628-87-5

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AT 125260-53-9

RX(32) RCT AT 125260-53-9

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

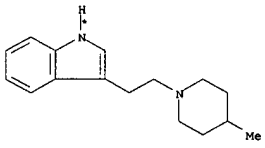
STAGE(1)
RGT AX 7722-84-1 H2O2

STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

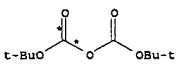
STAGE(3)
RGT I 151-50-8 KCN

PRO AW 125260-56-2

RX(66) OF 137 COMPOSED OF RX(30), RX(33)
RX(66) AR + Z ===> AZ

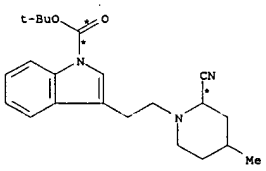


AR



Z

2 STEPS



AZ
YIELD 56%

RX(30) RCT AR 125260-52-8

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO AU 125260-54-0

RX(33) RCT AU 125260-54-0

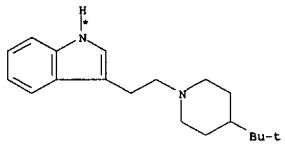
STAGE(1)
RGT AX 7722-84-1 H2O2

STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

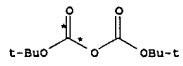
STAGE(3)
RGT I 151-50-8 KCN

PRO AZ 125260-57-3

RX(67) OF 137 COMPOSED OF RX(31), RX(34)
RX(67) AS + Z ===> AO

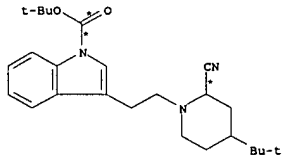


AS



Z

2 STEPS



AO
YIELD 62%

RX(31) RCT AS 58534-26-2

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AV 125260-55-1

RX(34) RCT AV 125260-55-1

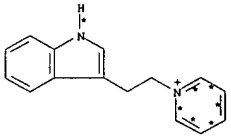
STAGE(1)
RGT AX 7722-84-1 H2O2

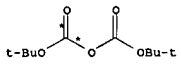
STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

STAGE(3)
RGT I 151-50-8 KCN

PRO AO 125260-58-4

RX(107) OF 137 COMPOSED OF RX(26), RX(29), RX(32)
RX(107) G + Z ===> AW

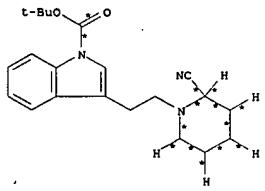




G Z

3 STEPS

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AW
YIELD 55%

RX(26) RCT G 50676-26-1
RGT V 1333-74-0 H2
PRO AQ 26628-87-5
CAT 1314-15-4 PtO2

RX(29) RCT AQ 26628-87-5

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AT 125260-53-9

RX(32) RCT AT 125260-53-9

STAGE(1)
RGT AX 7722-84-1 H2O2

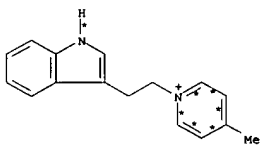
STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

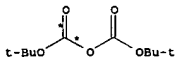
STAGE(3)
RGT I 151-50-8 KCN

PRO AW 125260-56-2

RX(109) OF 137 COMPOSED OF RX(27), RX(30), RX(33)
RX(109) C + Z ===> AZ

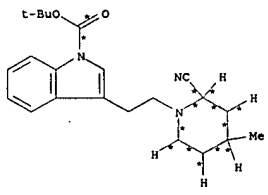
L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)





C Z

3 STEPS



AZ
YIELD 56%

RX(27) RCT C 24716-26-5
RGT V 1333-74-0 H2
PRO AR 125260-52-8
CAT 1314-15-4 PtO2

RX(30) RCT AR 125260-52-8

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AU 125260-54-0

RX(33) RCT AU 125260-54-0

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

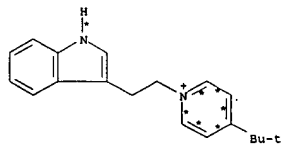
STAGE(1)
RGT AX 7722-84-1 H2O2

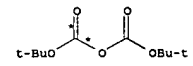
STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

STAGE(3)
RGT I 151-50-8 KCN

PRO AZ 125260-57-3

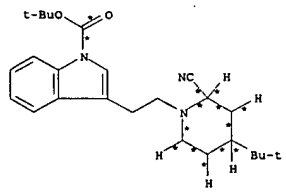
RX(111) OF 137 COMPOSED OF RX(28), RX(31), RX(34)
RX(111) E + Z ===> AO





E Z

3 STEPS



AO
YIELD 62%

L2 ANSWER 17 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(28) RCT E 125285-65-6
RGT V 1333-74-0 H2
PRO AS 58534-26-2
CAT 1314-15-4 PtO2

RX(31) RCT AS 58534-26-2

STAGE(1)
RGT AB 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7732-18-5 Water

STAGE(2)
RCT Z 24424-99-5
SOL 108-88-3 PhMe

PRO AV 125260-55-1

RX(34) RCT AV 125260-55-1

STAGE(1)
RGT AX 7722-84-1 H2O2

STAGE(2)
RGT AY 407-25-0 (CF3CO)2O

STAGE(3)
RGT I 151-50-8 KCN

PRO AO 125260-58-4

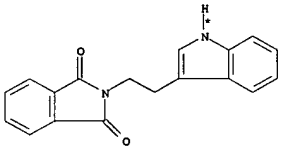
L2 ANSWER 18 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 111:56746 CASREACT
TITLE: Photochemistry of the phthalimide system. XLI. Intramolecular photoreactions of phthalimide-alkene systems. Oxetane formation of N-(ω-indol-3-ylalkyl)phthalimides
AUTHOR(S): Takechi, Haruko; Machida, Minoru; Kanaoka, Yuichi
CORPORATE SOURCE: Fac. Pharm. Sci., Higashi-Nippon-Gakuen Univ., Hokkaido, 061-02, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(8), 2853-63
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

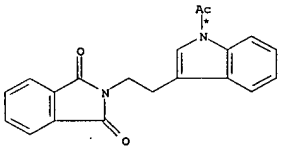
AB Upon irradiation in acetone, N-(ω-indol-3-ylalkyl)phthalimides I (n = 2-5) underwent intramol. Paterno-Buchi reaction to give oxeto[2,3-b]indoles (II) or their ring-opened products. However, N-(ω-indol-2-ylalkyl)phthalimides III (n = 2, 3) yielded not the oxetane, but the N-deacetylated compds. IV.

RX(17) OF 72 ...AP ===> D...



AP (17)

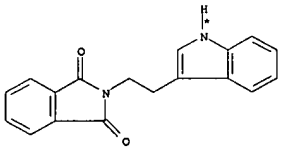
L2 ANSWER 18 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



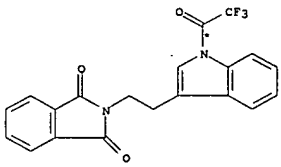
D

RX(17) RCT AP 15741-71-6
RGT AL 108-24-7 Ac2O, AM 584-08-7 K2CO3
PRO D 85632-71-9
SOL 68-12-2 DMF

RX(34) OF 72 ...AP ===> N...



AP (34)

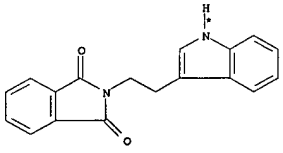


N
YIELD 60%

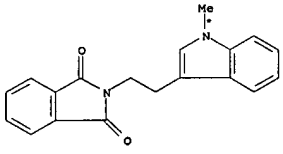
L2 ANSWER 18 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(34) RCT AP 15741-71-6
RGT AM 584-08-7 K2CO3, BK 407-25-0 (CF3CO)2O
PRO N 85616-85-9
SOL 68-12-2 DMF

RX(35) OF 72 ...AP ===> BL



AP (35)



BL
YIELD 90%

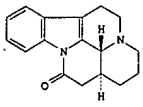
RX(35) RCT AP 15741-71-6

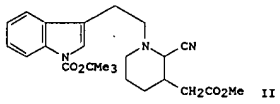
STAGE(1)
RGT BM 7693-26-7 KH
SOL 109-99-9 THF

STAGE(2)
RGT AI 74-88-4 MeI

PRO BL 70369-20-9

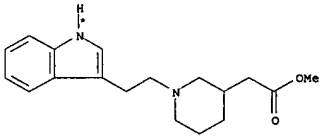
L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 110:95591 CASREACT
TITLE: Synthesis of compounds in the eburnamonine-homoeburnamonine series
AUTHOR(S): Jokela, Reija; Karvinen, Esko; Tolvanen, Arto; Lounasmaa, Mauri
CORPORATE SOURCE: Lab. Org. Bbioorg. Chem., Tech. Univ. Helsinki, Espoo, SF-02150, Finland
SOURCE: Tetrahedron (1988), 44(8), 2367-75
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

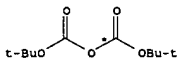

I


II

AB Six different lactams of the desethyleburnamonine-homoeburnamonine series, e.g. I, were synthesized. Thus, the piperidinoethylindole II, prepared in 3 steps from Me 3-pyridylacetate and tryptophyl bromide, was cyclized by AgBF4 to give 70% I. Complete 13C NMR data are presented for these compds., as well as for their precursors. Special attention is paid to their C(20)-C(21) stereochem.

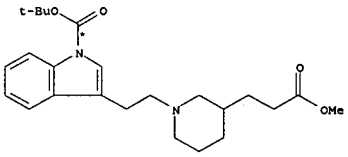
RX(3) OF 66 ...B + G ===> H...


B


G

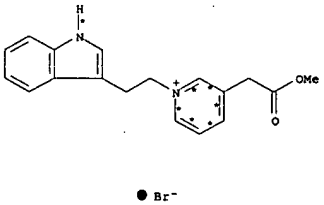
(3)

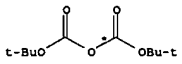
L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)


M
YIELD 98%

RX(4) RCT F 119100-73-1
STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe
STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe
PRO M 119100-75-3

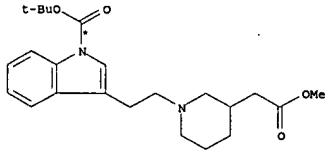
RX(20) OF 66 COMPOSED OF RX(1), RX(3)
RX(20) A + G ===> H


A


G

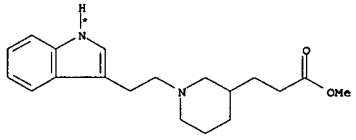
2 STEPS

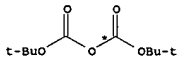
L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)


H
YIELD 98%

RX(3) RCT B 50676-27-2
STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe
STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe
PRO H 119100-74-2

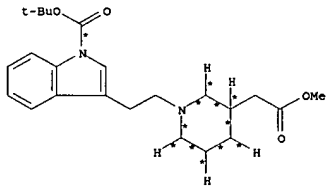
RX(4) OF 66 ...F + G ===> M...


F


G

(4)

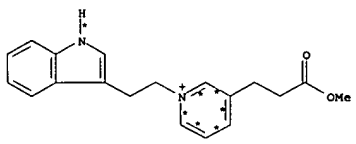
L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

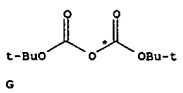

H
YIELD 98%

RX(1) RCT A 14996-87-3
RGT C 1333-74-0 H2
PRO B 50676-27-2
CAT 1314-15-4 PtO2

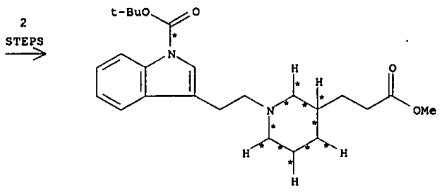
RX(3) RCT B 50676-27-2
STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe
STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe
PRO H 119100-74-2

RX(21) OF 66 COMPOSED OF RX(2), RX(4)
RX(21) E + G ===> M


E


G

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



M
YIELD 98%

RX(2) RCT E 89486-66-8
RGT C 1333-74-0 H2
PRO F 119100-73-1
CAT 1314-15-4 PtO2

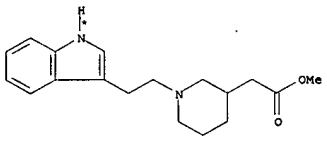
RX(4) RCT F 119100-73-1

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

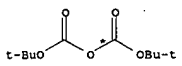
STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO M 119100-75-3

RX(22) OF 66 COMPOSED OF RX(3), RX(5)
RX(22) B + G ===> N

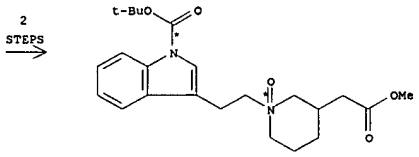


B



G

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



N
YIELD 90%

RX(3) RCT B 50676-27-2

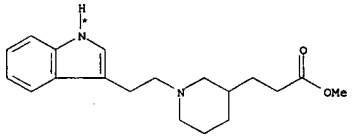
STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

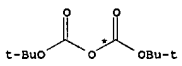
PRO H 119100-74-2

RX(5) RCT H 119100-74-2
RGT O 7722-84-1 H2O2
PRO N 119137-70-1
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(23) OF 66 COMPOSED OF RX(4), RX(6)
RX(23) F + G ===> R

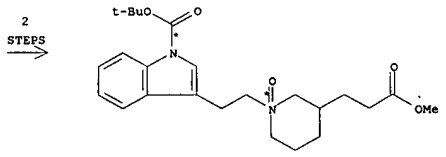


F



G

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



R
YIELD 90%

RX(4) RCT F 119100-73-1

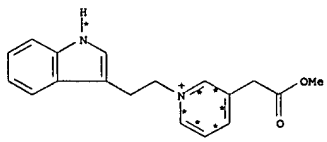
STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO M 119100-75-3

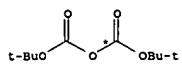
RX(6) RCT M 119100-75-3
RGT O 7722-84-1 H2O2
PRO R 119100-83-3
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(34) OF 66 COMPOSED OF RX(1), RX(3), RX(5)
RX(34) A + G ===> N



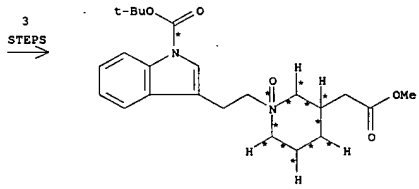
● Br⁻

A



G

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



N
YIELD 90%

RX(1) RCT A 14996-87-3
RGT C 1333-74-0 H2
PRO B 50676-27-2
CAT 1314-15-4 PtO2

RX(3) RCT B 50676-27-2

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

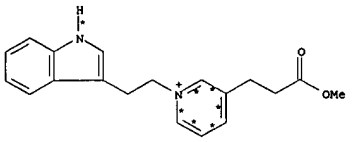
STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO H 119100-74-2

RX(5) RCT H 119100-74-2
RGT O 7722-84-1 H2O2
PRO N 119137-70-1
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

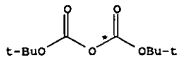
RX(36) OF 66 COMPOSED OF RX(2), RX(4), RX(6)
RX(36) E + G ===> R

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



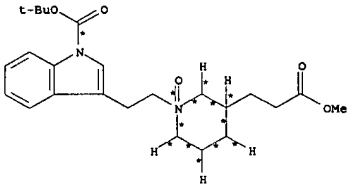
● Br⁻

E



G

3 STEPS



R
YIELD 90%

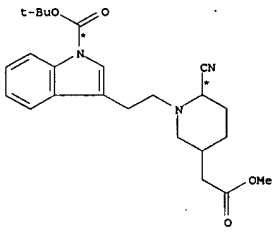
RX(2) RCT E 89486-66-8
RGT C 1333-74-0 H2
PRO F 119100-73-1
CAT 1314-15-4 PtO2

RX(4) RCT F 119100-73-1

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AW
YIELD 86%(50)

RX(3) RCT B 50676-27-2

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO H 119100-74-2

RX(5) RCT H 119100-74-2
RGT O 7722-84-1 H2O2
PRO N 119137-70-1
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(18) RCT N 119137-70-1

STAGE(1)
RGT BA 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT BB 151-50-8 KCN
SOL 7732-18-5 Water

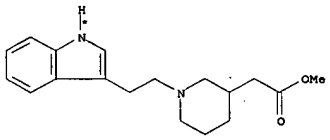
PRO S 119100-76-4, AW 119137-69-8

RX(39) OF 66 COMPOSED OF RX(1), RX(3), RX(5), RX(18)
RX(39) 2 A + 2 G ===> S + AW

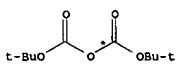
L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
PRO M 119100-75-3

RX(6) RCT M 119100-75-3
RGT O 7722-84-1 H2O2
PRO R 119100-83-3
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(38) OF 66 COMPOSED OF RX(3), RX(5), RX(18)
RX(38) 2 B + 2 G ===> S + AW

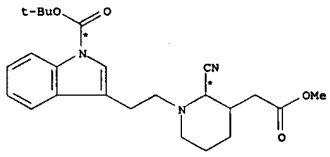


2 B



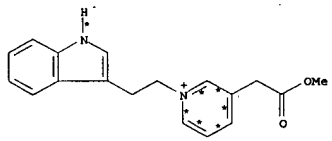
2 G

3 STEPS



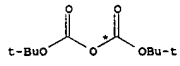
S
YIELD 86%(50)

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



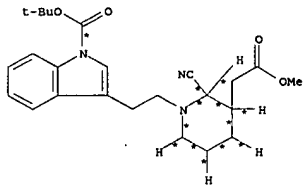
● Br⁻

2 A



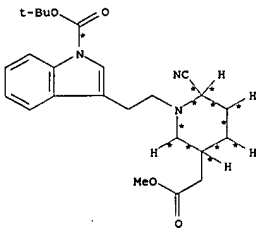
2 G

4 STEPS



S
YIELD 86%(50)

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AW
YIELD 86%(50)

RX(1) RCT A 14996-87-3
RGT C 1333-74-0 H2
PRO B 50676-27-2
CAT 1314-15-4 PtO2

RX(3) RCT B 50676-27-2

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO H 119100-74-2

RX(5) RCT H 119100-74-2
RGT O 7722-84-1 H2O2
PRO N 119137-70-1
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

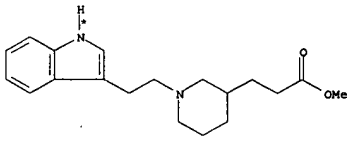
RX(18) RCT N 119137-70-1

STAGE(1)
RGT BA 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

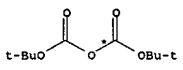
STAGE(2)
RGT BB 151-50-8 KCN
SOL 7732-18-5 Water

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
PRO S 119100-76-4, AW 119137-69-8

RX(40) OF 66 COMPOSED OF RX(4), RX(6), RX(19)
RX(40) 2 F + 2 G ===> W + AY

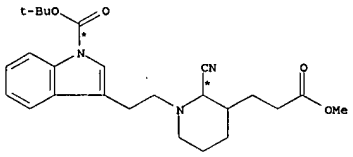


2 F



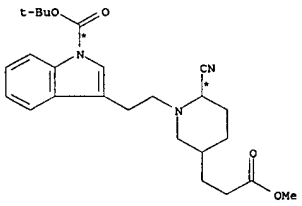
2 G

3
STEPS



W
YIELD 91%(50)

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AY
YIELD 91%(50)

RX(4) RCT F 119100-73-1

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO M 119100-75-3

RX(6) RCT M 119100-75-3
RGT O 7722-84-1 H2O2
PRO R 119100-83-3
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(19) RCT R 119100-83-3

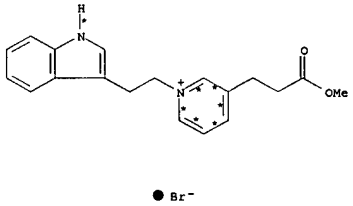
STAGE(1)
RGT BA 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT BB 151-50-8 KCN
SOL 7732-18-5 Water

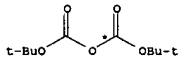
PRO W 119100-77-5, AY 119100-82-2

RX(41) OF 66 COMPOSED OF RX(2), RX(4), RX(6), RX(19)
RX(41) 2 E + 2 G ===> W + AY

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

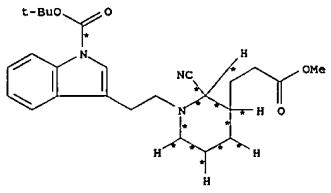


2 E



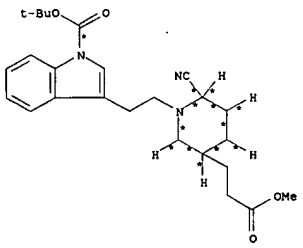
2 G

4
STEPS



W
YIELD 91%(50)

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AY
YIELD 91%(50)

RX(2) RCT E 89486-66-8
RGT C 1333-74-0 H2
PRO F 119100-73-1
CAT 1314-15-4 PtO2

RX(4) RCT F 119100-73-1

STAGE(1)
RGT I 32503-27-8 Bu4N.HSO4, J 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)
RCT G 24424-99-5
SOL 108-88-3 PhMe

PRO M 119100-75-3

RX(6) RCT M 119100-75-3
RGT O 7722-84-1 H2O2
PRO R 119100-83-3
SOL 7732-18-5 Water, 67-66-3 CHCl3, 67-56-1 MeOH

RX(19) RCT R 119100-83-3

STAGE(1)
RGT BA 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

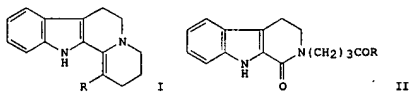
STAGE(2)
RGT BB 151-50-8 KCN
SOL 7732-18-5 Water

L2 ANSWER 19 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO W 119100-77-5, AY 119100-82-2

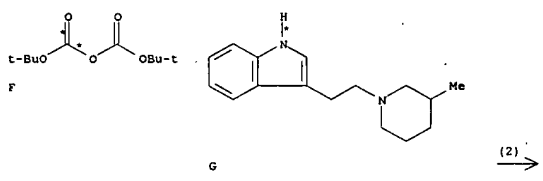
L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 109:129408 CASREACT
TITLE: A mild novel synthesis of simple 1-oxo-β-carbolines
AUTHOR(S): Jokela, Reija; Lounasmaa, Mauri
CORPORATE SOURCE: Lab. Org. Bioorg. Chem., Tech. Univ. Helsinki, Espoo, SF-02150, Finland
SOURCE: Tetrahedron (1987), 43(24), 6001-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

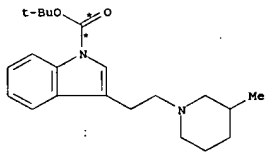


AB A new route using very mild reaction conditions, i.e. heating in EtOH, is described for the transformation of indoloquinolizidines I (R = Me, Et) to the 1-oxo-1,2,3,4-tetrahydro-β-carbolines II.

RX(2) OF 41 ...F + G ===> H...



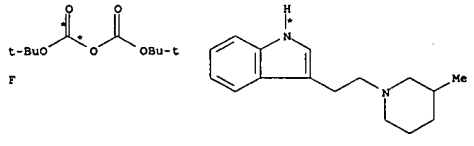
L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



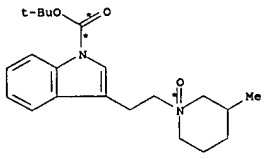
H
YIELD 98%

RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(10) OF 41 COMPOSED OF RX(2), RX(3)
RX(10) F + G ===> K



L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

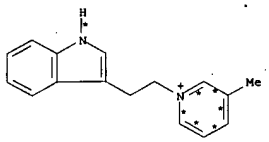


K
YIELD 91%

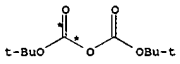
RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(3) RCT H 116171-57-4
RGT L 7722-84-1 H2O2
PRO K 116171-60-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(14) OF 41 COMPOSED OF RX(5), RX(2)
RX(14) T + F ===> H



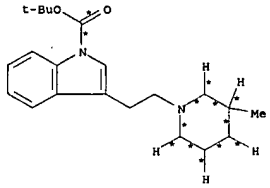
T



F

2
STEPS

L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

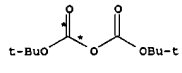


H
YIELD 98%

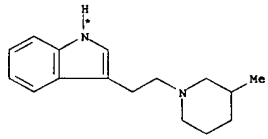
RX(5) RCT T 24716-23-2
RGT U 1333-74-0 H2
PRO G 13427-00-4
CAT 1314-15-4 PtO2
SOL 67-56-1 MeOH

RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(18) OF 41 COMPOSED OF RX(2), RX(3), RX(7)
RX(18) 2 F + 2 G ===> W + X



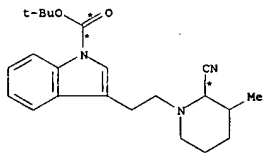
2 F



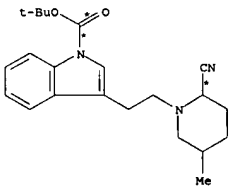
2 G

3
STEPS

L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



W



X

RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(3) RCT H 116171-57-4
RGT L 7722-84-1 H2O2
PRO K 116171-60-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(7) RCT K 116171-60-9

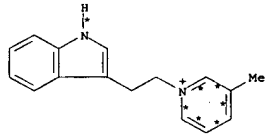
STAGE(1)
RGT R 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT AB 151-50-8 KCN
SOL 7732-18-5 Water

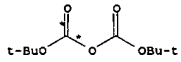
PRO W 116171-59-5, X 116171-59-6
NTE 73% overall

RX(19) OF 41 COMPOSED OF RX(5), RX(2), RX(3), RX(7)
RX(19) 2 T + 2 F ===> W + X

L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

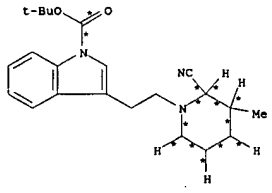


2 T

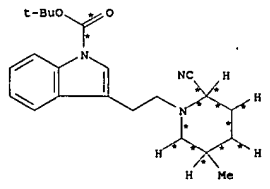


2 F

4
STEPS



W



X

RX(5) RCT T 24716-23-2

L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT U 1333-74-0 H2
PRO G 13427-00-4
CAT 1314-15-4 PtO2
SOL 67-56-1 MeOH

RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(3) RCT H 116171-57-4
RGT L 7722-84-1 H2O2
PRO K 116171-60-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

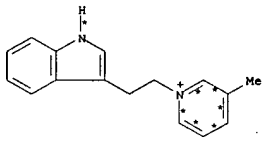
RX(7) RCT K 116171-60-9

STAGE(1)
RGT R 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

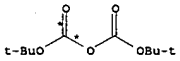
STAGE(2)
RGT AB 151-50-8 KCN
SOL 7732-18-5 Water

PRO W 116171-58-5, X 116171-59-6
NTE 73% overall

RX(22) OF 41 COMPOSED OF RX(5), RX(2), RX(3)
RX(22) T + F ===> K



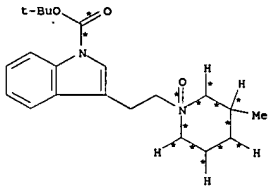
T



F

L2 ANSWER 20 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

3 STEPS



K
YIELD 91%

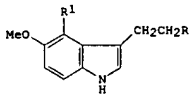
RX(5) RCT T 24716-23-2
RGT U 1333-74-0 H2
PRO G 13427-00-4
CAT 1314-15-4 PtO2
SOL 67-56-1 MeOH

RX(2) RCT F 24424-99-5, G 13427-00-4
RGT I 32503-27-8 Bu4N.HSO4
PRO H 116171-57-4
SOL 108-88-3 PhMe

RX(3) RCT H 116171-57-4
RGT L 7722-84-1 H2O2
PRO K 116171-60-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

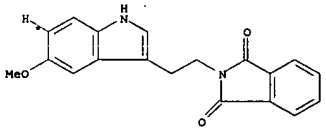
ACCESSION NUMBER: 109:37706 CASREACT
TITLE: Indole derivatives. 129. Synthesis of disubstituted tryptamines by nitration of 5-methoxy-N-phthalyltryptamines
AUTHOR(S): Petrunin, I. A.; Vinograd, L. H.; Przhiyalgovskaya, N.
M.; Suvorov, N. N.
CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987), (8), 1050-3
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

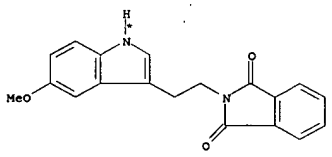
AB Nitration of 5-methoxy-N-phthalyltryptamine I (R = phthalimido, R1 = H) with HNO3 in AcOH gives mainly I (R1 = NO2). I (R1 = NH2, NHAc) were obtained from I (R1 = NO2).

RX(2) OF 19 ...4 C ===> D + E + F + G...

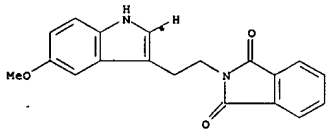


C

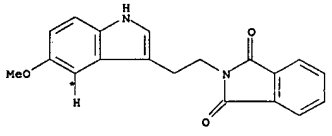
L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



C

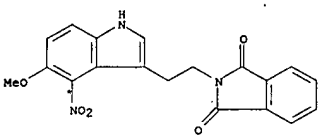


C

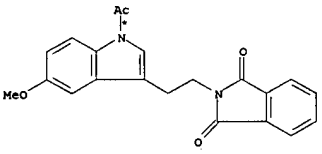


C (2)

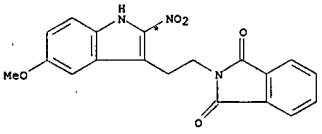
L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



D
YIELD 42%

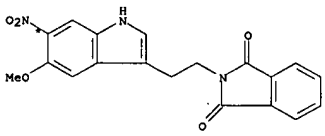


E
YIELD 5%



F

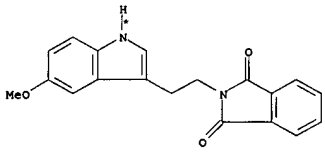
L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



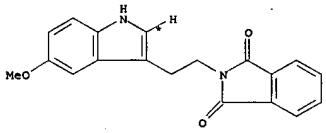
G
YIELD 6%

RX(2) RCT C 55747-66-5
RGT H 7697-37-2 HNO3
PRO D 115168-34-8, E 115168-35-9, F 115168-36-0, G 115168-37-1
SOL 64-19-7 AcOH

RX(3) OF 19 ...2 C + 2 J ===> E + K

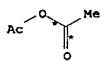


C



C

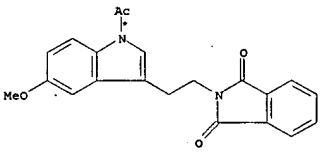
J



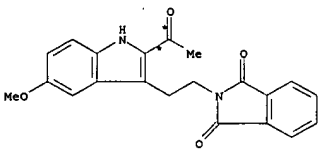
J

L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

(3)



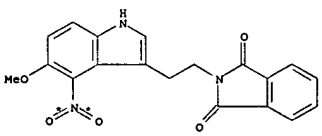
E
YIELD 9%



K
YIELD 26%

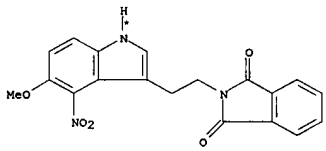
RX(3) RCT C 55747-66-5, J 108-24-7
PRO E 115168-35-9, K 115168-38-2
CAT 10034-81-8 Mg(ClO4)2

RX(6) OF 19 ...2 D + 2 J ===> T + U



D

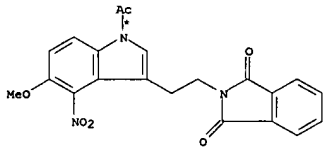
L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



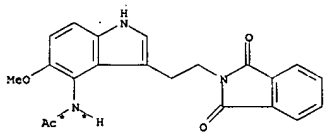
D

2 J

(6)



T
YIELD 12%



U
YIELD 34%

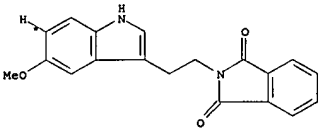
RX(6) RCT D 115168-34-8

STAGE(1)
RGT Q 1333-74-0 H2
CAT 7440-02-0 Ni
SOL 68-12-2 DMF

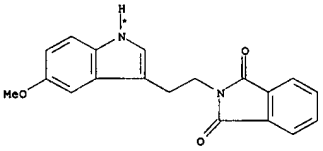
STAGE(2)
RCT J 108-24-7

L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
PRO T 115168-42-8, U 115168-41-7

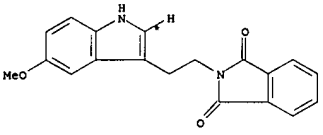
RX(13) OF 19 COMPOSED OF RX(2), RX(6)
RX(13) 5 C + 2 J ===> T + U



C

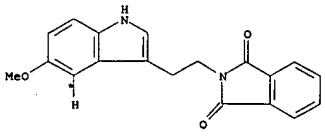


C

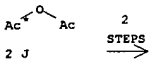


C

L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

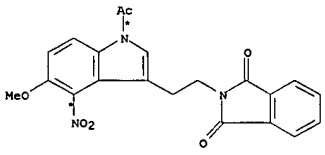


2 C

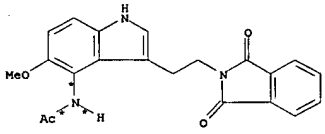


2 J

2 STEPS



T
YIELD 12%



U
YIELD 34%

RX(2) RCT C 55747-66-5
RGT H 7697-37-2 HNO3
PRO D 115168-34-8, E 115168-35-9, F 115168-36-0, G 115168-37-1
SOL 64-19-7 AcOH

RX(6) RCT D 115168-34-8

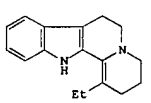
STAGE(1)

L2 ANSWER 21 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
RGT Q 1333-74-0 H2
CAT 7440-02-0 Ni
SOL 68-12-2 DMF

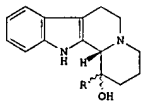
STAGE(2)
RCT J 108-24-7

PRO T 115168-42-8, U 115168-41-7

L2 ANSWER 22 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 108:204859 CASREACT
TITLE: Novel applications of the modified Polonovski reaction. IX. New route to Wenkert's enamine
AUTHOR(S): Lounasmaa, Mauri; Karvinen, Esko; Koskinen, Ari; Jokela, Reija
CORPORATE SOURCE: Lab. Org. Bioorg. Chem., Tech. Univ. Helsinki, Espoo, SF-02150, Finland
SOURCE: Tetrahedron (1987), 43(9), 2135-46
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



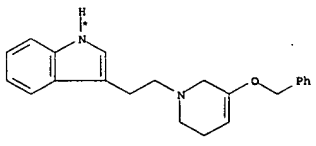
I



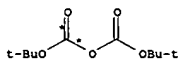
II

AB A practical synthetic entry to Wenkert's enamine (I) employing the modified Polonovski reaction is described. Complete 13C NMR spectral data of I is presented. Conformational anal. of the intermediate 1-hydroxy- and 1-ethyl-1-hydroxyinodolquinolizidines II (R = H, Et) based on simple but reliable 13C NMR spectral correlations is presented.

RX(4) OF 62 ...I + L ===> M...



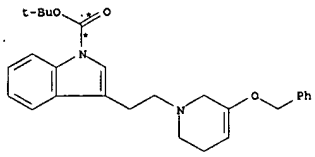
I



L

(4)

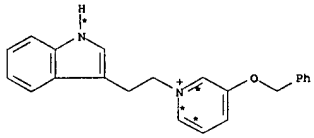
L2 ANSWER 22 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



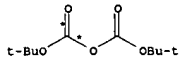
M
YIELD 90%

RX(4) RCT I 76509-19-8, L 24424-99-5
RGT N 1122-58-3 4-DMAP
PRO M 114495-25-9
SOL 75-09-2 CH2Cl2

RX(14) OF 62 COMPOSED OF RX(3), RX(4)
RX(14) G + L ===> M



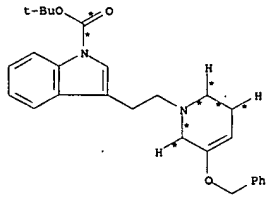
G



L

L2 ANSWER 22 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2 STEPS

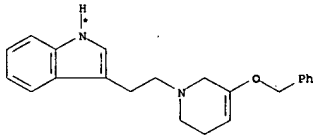


M
YIELD 90%

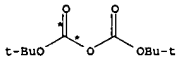
RX(3) RCT G 76509-18-7
RGT J 16940-66-2 NaBH4
PRO I 76509-19-8
SOL 64-17-5 EtOH

RX(4) RCT I 76509-19-8, L 24424-99-5
RGT N 1122-58-3 4-DMAP
PRO M 114495-25-9
SOL 75-09-2 CH2Cl2

RX(15) OF 62 COMPOSED OF RX(4), RX(5)
RX(15) I + L ===> P



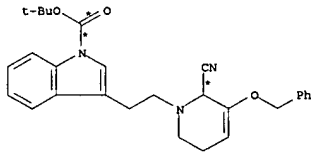
I



L

2 STEPS

L2 ANSWER 22 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



P
YIELD 100%

RX(4) RCT I 76509-19-8, L 24424-99-5
RGT N 1122-58-3 4-DMAP
PRO M 114495-25-9
SOL 75-09-2 CH2Cl2

RX(5) RCT M 114495-25-9

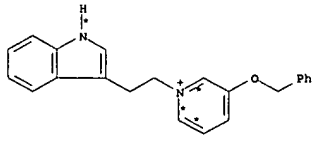
STAGE(1)
RGT Q 937-14-4 MCPBA
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT R 407-25-0 (CF3CO)2O

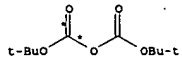
STAGE(3)
RGT S 151-50-8 KCN
SOL 7732-18-5 Water

PRO P 114495-24-8

RX(25) OF 62 COMPOSED OF RX(3), RX(4), RX(5)
RX(25) G + L ===> P



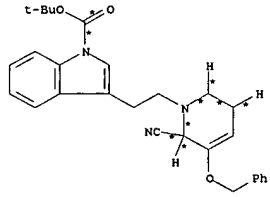
G



L

L2 ANSWER 22 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

3 STEPS



P
YIELD 100%

RX(3) RCT G 76509-18-7
RGT J 16940-66-2 NaBH4
PRO I 76509-19-8
SOL 64-17-5 EtOH

RX(4) RCT I 76509-19-8, L 24424-99-5
RGT N 1122-58-3 4-DMAP
PRO M 114495-25-9
SOL 75-09-2 CH2Cl2

RX(5) RCT M 114495-25-9

STAGE(1)
RGT Q 937-14-4 MCPBA
SOL 75-09-2 CH2Cl2

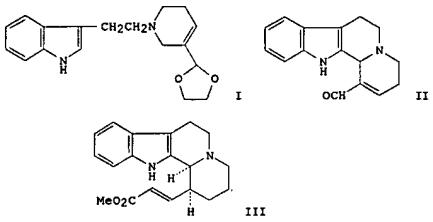
STAGE(2)
RGT R 407-25-0 (CF3CO)2O

STAGE(3)
RGT S 151-50-8 KCN
SOL 7732-18-5 Water

PRO P 114495-24-8

L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

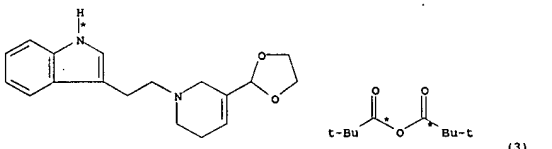
ACCESSION NUMBER: 108:56422 CASREACT
TITLE: Nitrogen assisted acetal ring cleavage. Part III. Synthesis and reactions of 1-formyl-3,4,6,7,12,12b-hexahydroindolo[2,3-a]quinolizine
AUTHOR(S): Tolvanen, Arto; Lounasmaa, Mauri
CORPORATE SOURCE: Lab. Org. Biocrg. Chem., Tech. Univ. Helsinki, Espoo, SF-02150, Finland
SOURCE: Tetrahedron (1987), 43(6), 1123-7
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II III

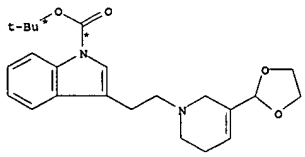
AB N-Protection followed by oxidation and cyclization of indole I gave indoloquinolizine II. II was converted to indoloquinolizineacrylate III, which can be used as intermediate for the synthesis of eburnamine-vincamine alkaloids.

RX(3) OF 68 ...D + G ===> H...



D G (3)

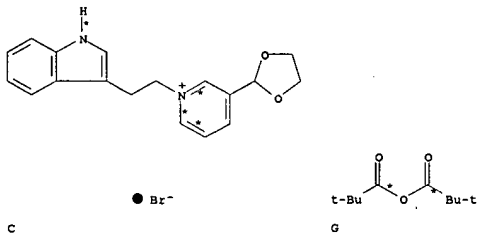
L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



H
YIELD 95%

RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

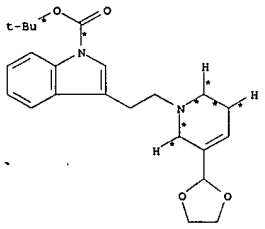
RX(16) OF 68 COMPOSED OF RX(2), RX(3)
RX(16) C + G ===> H



C G

L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2 STEPS

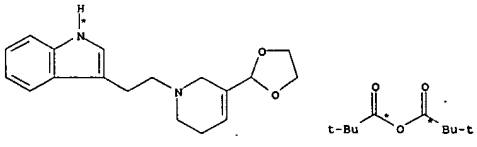


H
YIELD 95%

RX(2) RCT C 105702-50-9
RGT E 16940-66-2 NaBH4
PRO D 105688-95-7
SOL 64-17-5 EtOH

RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

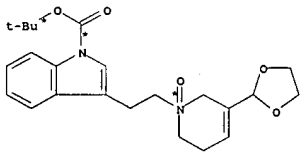
RX(17) OF 68 COMPOSED OF RX(3), RX(4)
RX(17) D + G ===> K



D G

L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2 STEPS

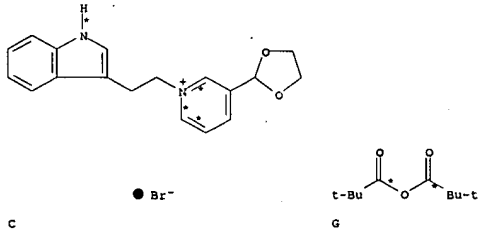


K
YIELD 91%

RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

RX(4) RCT H 112396-78-8
RGT L 7722-84-1 H2O2
PRO K 112396-79-9
SOL 7732-18-5 Water, 64-17-5 EtOH, 67-66-3 CHCl3

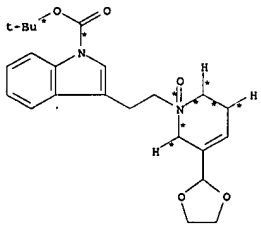
RX(28) OF 68 COMPOSED OF RX(2), RX(3), RX(4)
RX(28) C + G ===> K



C G

L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

3 STEPS



K
YIELD 91%

RX(2) RCT C 105702-50-9
RGT E 16940-66-2 NaBH4
PRO D 105688-95-7
SOL 64-17-5 EtOH

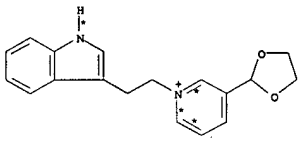
RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

RX(4) RCT H 112396-78-8
RGT L 7722-84-1 H2O2
PRO K 112396-79-9
SOL 7732-18-5 Water, 64-17-5 EtOH, 67-66-3 CHCl3

RX(30) OF 68 COMPOSED OF RX(3), RX(4), RX(5)
RX(30) D + G ===> O

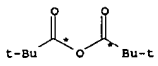
L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
SOL 75-09-2 CH2Cl2

RX(31) OF 68 COMPOSED OF RX(2), RX(3), RX(4), RX(5)
RX(31) C + G ===> O



● Br⁻

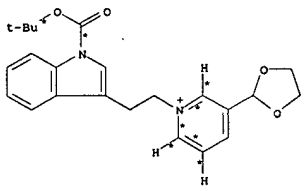
C



G

4 STEPS

O: CM 1

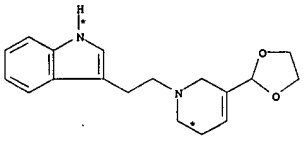


O: CM 2

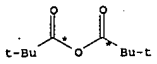
RX(2) RCT C 105702-50-9
RGT E 16940-66-2 NaBH4
PRO D 105688-95-7
SOL 64-17-5 EtOH

RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



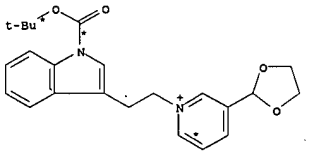
D



G

3 STEPS

O: CM 1



O: CM 2

RX(3) RCT D 105688-95-7, G 1538-75-6
PRO H 112396-78-8
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

RX(4) RCT H 112396-78-8
RGT L 7722-84-1 H2O2
PRO K 112396-79-9
SOL 7732-18-5 Water, 64-17-5 EtOH, 67-66-3 CHCl3

RX(5) RCT K 112396-79-9
RGT P 407-25-0 (CF3CO)2O
PRO O 112418-33-4

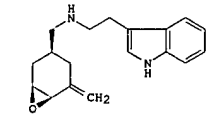
L2 ANSWER 23 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(4) RCT H 112396-78-8
RGT L 7722-84-1 H2O2
PRO K 112396-79-9
SOL 7732-18-5 Water, 64-17-5 EtOH, 67-66-3 CHCl3

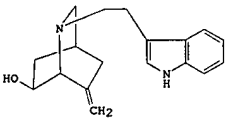
RX(5) RCT K 112396-79-9
RGT P 407-25-0 (CF3CO)2O
PRO O 112418-33-4
SOL 75-09-2 CH2Cl2

L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 105:191462 CASREACT
TITLE: Synthesis of optically active isoquinuclidines utilizing a diastereoselectivity control element
AUTHOR(S): Trost, Barry M.; Romero, Arthur G.
CORPORATE SOURCE: McElvain Lab. Org. Chem., Univ. Wisconsin-Madison, Madison, WI, 53706, USA
SOURCE: Journal of Organic Chemistry (1986), 51(12), 2332-42
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

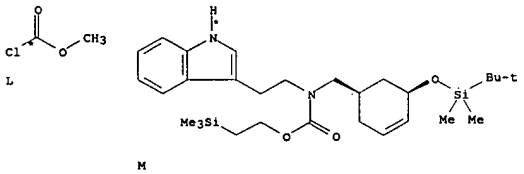


II

AB The development of a palladium-mediated cyclization via isomerization using a vinyl epoxide as an initiator and an amine as a terminator led to a facile cyclization to produce isoquinuclidines. The synthesis of the requisite cyclizaton precursor I from (-)-quinic acid led to the isoquinuclidine II in optically pure form. The substitution pattern of the resultant isoquinuclidine would allow further cyclization to either enantiomeric series of the iboga alkaloids. This "pseudo-meso" intermediate then can become a common intermediate to either ibogamine or catharanthine, the latter of particular importance in the synthesis of vinblastine analogs. The olefination of an epoxy ketone proceeds with high geometrical control.

RX(4) OF 305 ...L + M ===> N...

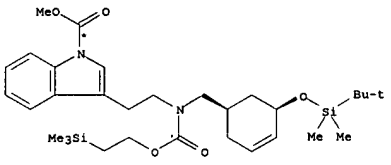
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



L

M

(4)

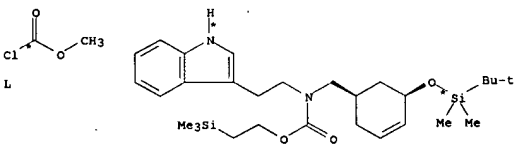


N

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(38) OF 305 COMPOSED OF RX(4), RX(5)
RX(38) L + M ===> Q

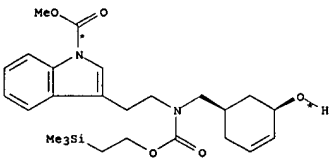
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



L

M

2
STEPS



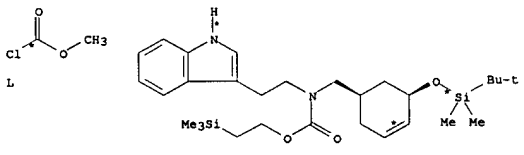
Q

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(72) OF 305 COMPOSED OF RX(4), RX(5), RX(6)
RX(72) L + M ===> T

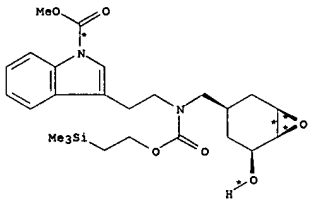
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



L

M

3
STEPS



T

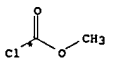
RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

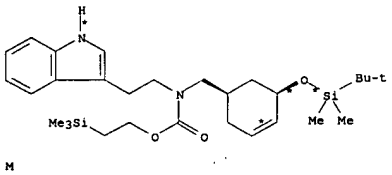
RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA
PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

RX(75) OF 305 COMPOSED OF RX(4), RX(5), RX(6), RX(7)
RX(75) L + M ===> W

L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

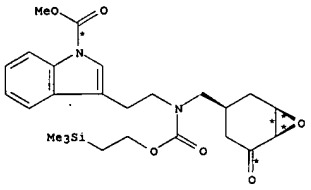


L



M

4
STEPS



W

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA
PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

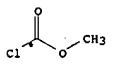
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

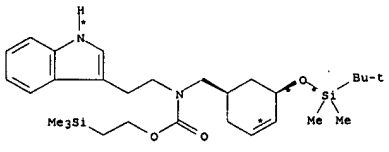
RX(7) RCT T 101932-70-1
RGT X 79-37-8 (COCl)2
PRO W 101917-41-3
SOL 75-09-2 CH2Cl2

RX(10) RCT AE 2065-66-9, W 101917-41-3
RGT AF 865-47-4 t-BuOK
PRO Y 101917-39-9
SOL 109-99-9 THF

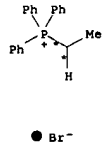
RX(132) OF 305 COMPOSED OF RX(4), RX(5), RX(6), RX(7), RX(34)
RX(132) L + M + CG ===> AI



L



M



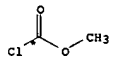
CG

5
STEPS

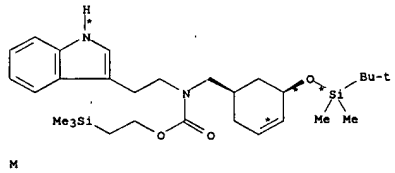
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(7) RCT T 101932-70-1
RGT X 79-37-8 (COCl)2
PRO W 101917-41-3
SOL 75-09-2 CH2Cl2

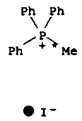
RX(131) OF 305 COMPOSED OF RX(4), RX(5), RX(6), RX(7), RX(10)
RX(131) L + M + AE ===> Y



L

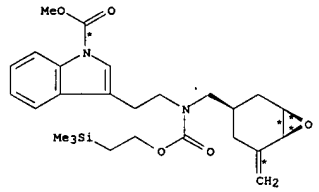


M



AE

5
STEPS



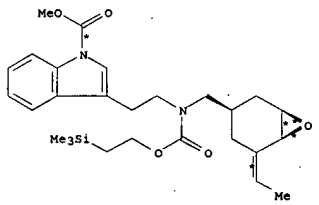
Y

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA

L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AI

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

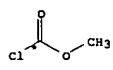
RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA
PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

RX(7) RCT T 101932-70-1
RGT X 79-37-8 (COCl)2
PRO W 101917-41-3
SOL 75-09-2 CH2Cl2

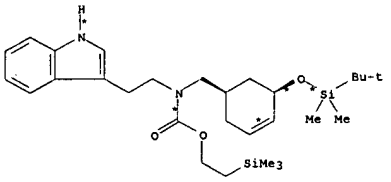
RX(34) RCT W 101917-41-3, CG 1530-32-1
RGT AF 865-47-4 t-BuOK
PRO AI 101917-44-6
SOL 109-99-9 THF

RX(147) OF 305 COMPOSED OF RX(4), RX(5), RX(6), RX(7), RX(34), RX(13)
RX(147) L + M + CG ===> AK

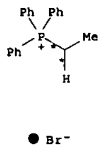


L

L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

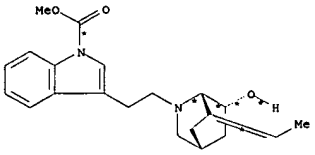


M



CG

6
STEPS



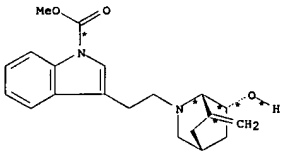
AK

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA
PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AG

RX(4) RCT L 79-22-1, M 101917-36-6
RGT O 7693-26-7 KH
PRO N 101917-37-7
SOL 109-99-9 THF

RX(5) RCT N 101917-37-7
RGT R 64-19-7 AcOH
PRO Q 101917-38-8
SOL 7732-18-5 Water, 109-99-9 THF

RX(6) RCT Q 101917-38-8
RGT U 937-14-4 MCPBA
PRO T 101932-70-1
SOL 75-09-2 CH2Cl2

RX(7) RCT T 101932-70-1
RGT X 79-37-8 (COCl)2
PRO W 101917-41-3
SOL 75-09-2 CH2Cl2

RX(10) RCT AE 2065-66-9, W 101917-41-3
RGT AF 865-47-4 t-BuOK
PRO Y 101917-39-9
SOL 109-99-9 THF

RX(8) RCT Y 101917-39-9
RGT AA 429-41-4 Bu4N.F
PRO Z 101917-42-4
SOL 75-05-8 MeCN

RX(11) RCT Z 101917-42-4
PRO AG 101917-43-5
CAT 14221-01-3 Pd(PPh3)4
SOL 109-99-9 THF

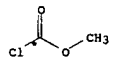
L2 ANSWER 24 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(7) RCT T 101932-70-1
RGT X 79-37-8 (COCl)2
PRO W 101917-41-3
SOL 75-09-2 CH2Cl2

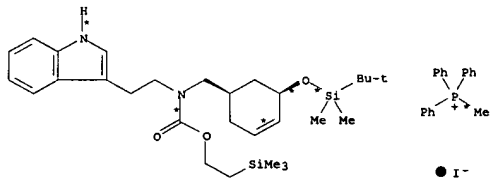
RX(34) RCT W 101917-41-3, CG 1530-32-1
RGT AF 865-47-4 t-BuOK
PRO AI 101917-44-6
SOL 109-99-9 THF

RX(13) RCT AI 101917-44-6
PRO AK 101917-45-7
CAT 14221-01-3 Pd(PPh3)4
SOL 109-99-9 THF

RX(156) OF 305 COMPOSED OF RX(4), RX(5), RX(6), RX(7), RX(10), RX(8), RX(11)
RX(156) L + M + AE ===> AG



L



M

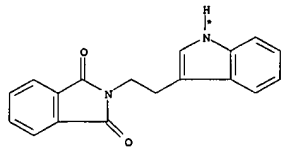
AE

7
STEPS

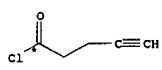
L2 ANSWER 25 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 104:224804 CASREACT
TITLE: Cobalt-mediated [2 + 2 + 2] cycloadditions of alkynes to the indole 2,3-double bond: an extremely facile entry into the novel 4a,9a-dihydro-9H-carbazole nucleus
AUTHOR(S): Grotjahn, Douglas B.; Vollhardt, K. Peter C.
CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Journal of the American Chemical Society (1986), 108(8), 2091-3
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB η-Cyclopentadienyl cobalt (CpCo) reagent mediates the [2+2+2]cycloaddn. of the indole Me, etc., Z = O, H2; R1 = H, (CH2)4C.tplbond.CH) complexed fused polyheterocycles with stereo- and regiospecificity. Thus, treating indoles I (n = 2,3; R = H Me; Z = O or H2) with (Me3SiC.tplbond.)2 in the presence CpCo reagent cycloadducts II, along with cyclobutadiene compds. III.

RX(6) OF 42 L + B ===> M...

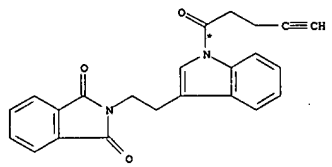


L



B

(6)

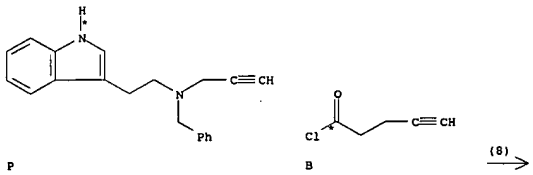


M

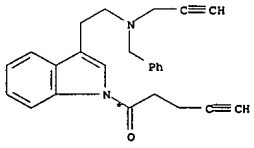
RX(6) RCT L 15741-71-6, B 55183-44-3
PRO M 101079-43-0

L2 ANSWER 25 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(8) OF 42 P + B ===> Q...



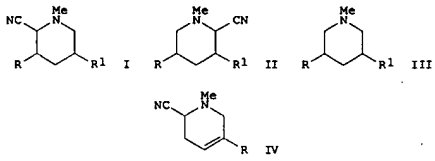
P B (8)



Q

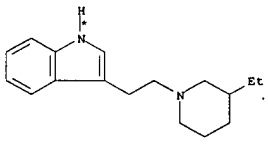
RX(8) RCT P 62002-15-7, B 55183-44-3
PRO Q 101079-45-2

L2 ANSWER 26 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 104:129755 CASREACT
TITLE: Carbon-13 NMR spectral and stereochemical analysis of piperidine-derived α-amino nitriles
AUTHOR(S): Jokela, Reija; Tamminen, Tarja; Lounasmaa, Mauri
CORPORATE SOURCE: Dep. Chem., Tech. Univ. Helsinki, Espoo, SF-02150/15, Finland
SOURCE: Heterocycles (1985), 23(7), 1707-22
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

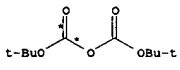


AB Cyanopiperidines I and II [R = Et, CH2CH2CO2Me, CH2CH(CO2Me)2, 2-dioxolanyl, R1 = H; R = CH2CH(CO2Me)2, R1 = Et] were prepared by Palonovski cyanation of the piperidines III; the cyanotetrahydropyridines IV [R = Et, CH2CH2CO2Me, CH2CH(CO2Me)2] were obtained by reductive cyanation of the corresponding N-methylpyridinium iodides. C-13 NMR spectra were determined for I, II, and IV, substituent effects for the cyano group in the different N heterocycles were determined, and conformation-NMR spectra correlations were made.

RX(36) OF 128 BR + BS ===> BT...

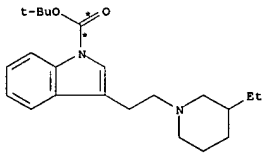


BR



BS (36)

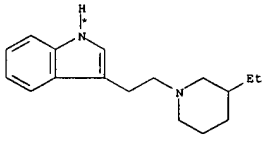
L2 ANSWER 26 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



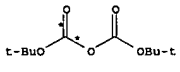
BT

RX(36) RCT BR 2671-39-8, BS 24424-99-5
RGT BU 1310-73-2 NaOH, BV 32503-27-8 Bu4N.HSO4
PRO BT 101026-08-8
SOL 7732-18-5 Water, 108-88-3 PhMe

RX(69) OF 128 COMPOSED OF RX(36), RX(37)
RX(69) BR + BS ===> BW



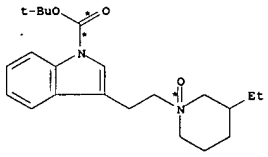
BR



BS

2 STEPS

L2 ANSWER 26 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

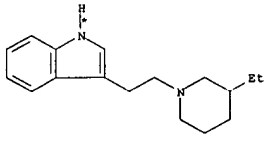


BW

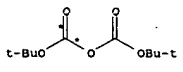
RX(36) RCT BR 2671-39-8, BS 24424-99-5
RGT BU 1310-73-2 NaOH, BV 32503-27-8 Bu4N.HSO4
PRO BT 101026-08-8
SOL 7732-18-5 Water, 108-88-3 PhMe

RX(37) RCT BT 101026-08-8
RGT AY 7722-84-1 H2O2
PRO BW 101026-09-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(106) OF 128 COMPOSED OF RX(36), RX(37), RX(38)
RX(106) 2 BR + 2 BS ===> BY + BZ



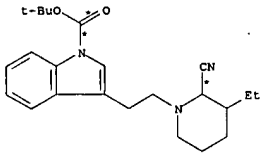
2 BR



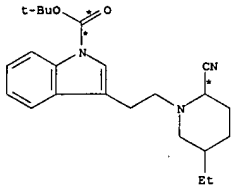
2 BS

3 STEPS

L2 ANSWER 26 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BY



BZ

RX(36) RCT BR 2671-39-8, BS 24424-99-5
RGT BU 1310-73-2 NaOH, BV 32503-27-8 Bu4N.HSO4
PRO BT 101026-08-8
SOL 7732-18-5 Water, 108-88-3 PhMe

RX(37) RCT BT 101026-08-8
RGT AY 7722-84-1 H2O2
PRO BW 101026-09-9
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(38) RCT BW 101026-09-9

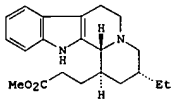
STAGE(1)
RGT BC 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT BD 151-50-8 KCN, BE 127-09-3 AcONa
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

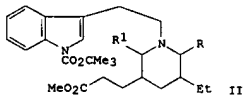
PRO BY 101026-10-2, BZ 101026-11-3

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 103:160750 CASREACT
TITLE: Novel applications of the modified Polonovski reaction
- VIII. Synthetic studies in the pseudovincamine series
AUTHOR(S): Jokela, Reija; Schuller, Siv; Lounasmaa, Mauri
CORPORATE SOURCE: Dep. Chem., Tech. Univ. Helsinki, Espoo, SF-02150/15, Finland
SOURCE: Heterocycles (1985), 23(7), 1751-7
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



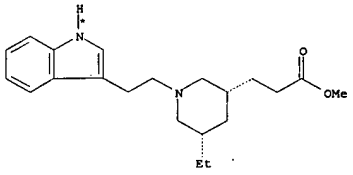
I



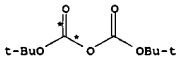
II

AB Indoloquinolizine I, a potential intermediate in the pseudovincamine series, was synthesized via Polonovski reaction of piperidinoethylindole II (R = R1 = H) to give II (R = H, R1 = cyano, R = cyano, R1 = H). The conformations of I were discussed.

RX(5) OF 36 ...K + M ===> N...



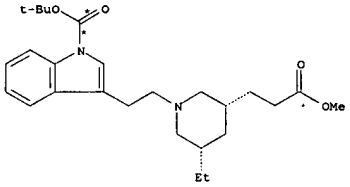
K



M

(5)

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



N

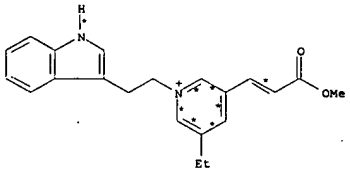
RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

STAGE(2)
SOL 108-88-3 PhMe

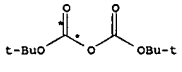
PRO N 98677-51-1

RX(12) OF 36 COMPOSED OF RX(4), RX(5)
RX(12) J + M ===> N



● Br⁻

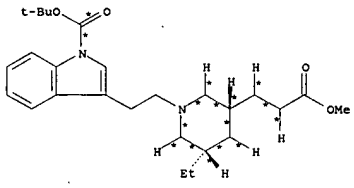
J



M

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2 STEPS



N

RX(4) RCT J 98664-65-4
RGT L 1333-74-0 H2
PRO K 98664-66-5

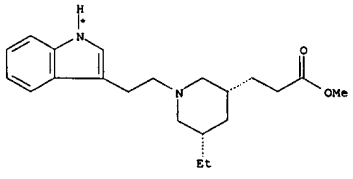
RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

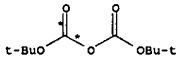
STAGE(2)
SOL 108-88-3 PhMe

PRO N 98677-51-1

RX(13) OF 36 COMPOSED OF RX(5), RX(6)
RX(13) K + M ===> S



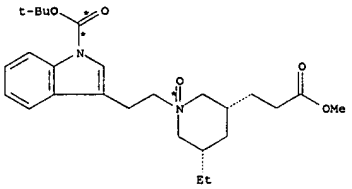
K



M

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2 STEPS



S

RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

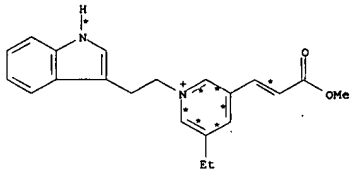
STAGE(2)
SOL 108-88-3 PhMe

PRO N 98677-51-1

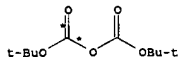
RX(6) RCT N 98677-51-1
RGT T 7722-84-1 H2O2
PRO S 98664-67-6
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(21) OF 36 COMPOSED OF RX(4), RX(5), RX(6)
RX(21) J + M ===> S

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

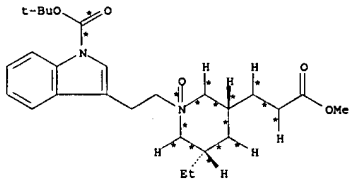


J



M

3 STEPS



S

RX(4) RCT J 98664-65-4
RGT L 1333-74-0 H2
PRO K 98664-66-5

RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

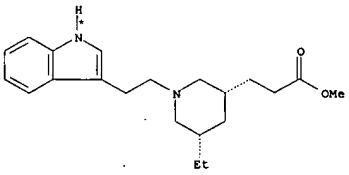
STAGE(2)
SOL 108-88-3 PhMe

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

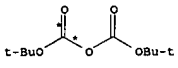
PRO N 98677-51-1

RX(6) RCT N 98677-51-1
RGT T 7722-84-1 H2O2
PRO S 98664-67-6
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(23) OF 36 COMPOSED OF RX(5), RX(6), RX(8)
RX(23) 2 K + 2 M ===> W + AB

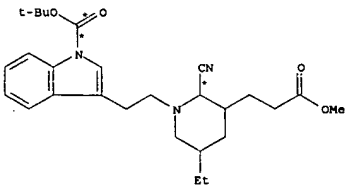


2 K



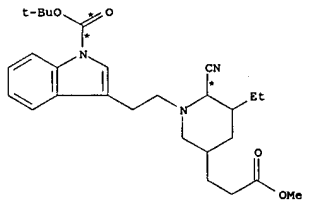
2 M

3 STEPS



W

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AB

RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

STAGE(2)
SOL 108-88-3 PhMe

PRO N 98677-51-1

RX(6) RCT N 98677-51-1
RGT T 7722-84-1 H2O2
PRO S 98664-67-6
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(8) RCT S 98664-67-6

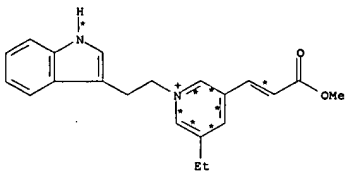
STAGE(1)
RGT AC 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2, 7440-37-1 Ar

STAGE(2)
RGT AD 151-50-8 KCN
SOL 7732-18-5 Water

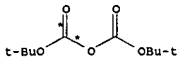
PRO W 98664-69-8, AB 98664-68-7

RX(24) OF 36 COMPOSED OF RX(4), RX(5), RX(6), RX(8)
RX(24) 2 J + 2 M ===> W + AB

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

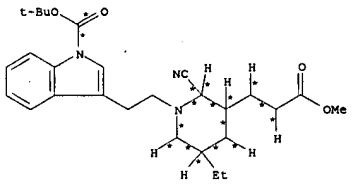


2 J



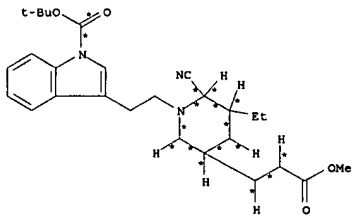
2 M

4 STEPS



W

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AB

RX(4) RCT J 98664-65-4
RGT L 1333-74-0 H2
PRO K 98664-66-5

RX(5) RCT K 98664-66-5, M 24424-99-5

STAGE(1)
RGT O 1310-73-2 NaOH
CAT 32503-27-8 Bu4N.HSO4
SOL 108-88-3 PhMe, 7440-37-1 Ar

STAGE(2)
SOL 108-88-3 PhMe

PRO N 98677-51-1

RX(6) RCT N 98677-51-1
RGT T 7722-84-1 H2O2
PRO S 98664-67-6
SOL 67-66-3 CHCl3, 67-56-1 MeOH

RX(8) RCT S 98664-67-6

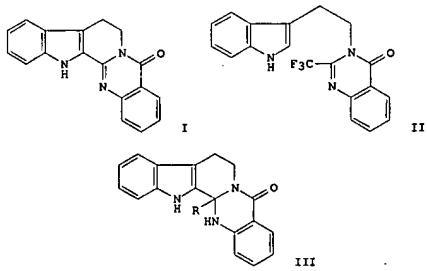
STAGE(1)
RGT AC 407-25-0 (CF3CO)2O
SOL 75-09-2 CH2Cl2, 7440-37-1 Ar

STAGE(2)
RGT AD 151-50-8 KCN
SOL 7732-18-5 Water

PRO W 98664-69-8, AB 98664-68-7

L2 ANSWER 27 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

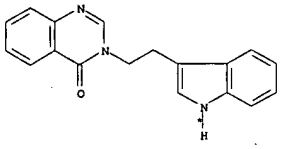
L2 ANSWER 28 OF 31 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 102:185337 CASREACT
TITLE: Studies of rutaecarpine and related quinazolinocarboline alkaloids
AUTHOR(S): Bergman, Jan; Bergman, Solveig
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SOURCE: Journal of Organic Chemistry (1985), 50(8), 1246-55
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Quniazolinocarboline alkaloids, e.g., rutaecaprine (I), can readily be synthesized by treating tryptamine with 2-(trifluoromethyl)-4H-3,1-benzoxazin-4-one which was generated in situ from (F3CCO)2O and 2H-3,1-benzoxazine-2,4(1H)-dione. The product formed, (indolylethyl)(trifluoromethyl)quinazolinone II, is then cyclized (HCl/HOAc) to (trifluoromethyl)dihydrorutaecarpine III (R = F3C), from which CF3H is eliminated by treatment with base. The sequence can conveniently be performed as a three-reaction one-pot procedure giving I in 99% yield within 3 h. The approach can readily be extended to the synthesis of evodiamine, 13,13b-dehydroevodiamine, and 13b,14-dihydrorutaecarpine (III, R = H). Thus treatment of 3-[2-(3-indolyl)ethyl]-4(3H)-quinazolinone with (F3CCO)2O gave (trifluoroacetyl)-13b,14-dihydrorutaecarpine, which was hydrolyzed to III (R = H).

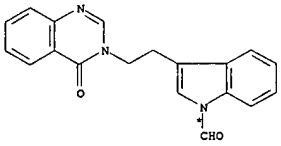
RX(11) OF 205 ...X ===> Z

L2 ANSWER 28 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



X

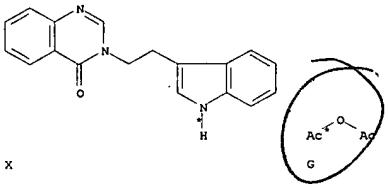
(11)



Z

RX(11) RCT X 60941-86-8
RGT AA 64-18-6 HCO2H
PRO Z 95274-45-6
SOL 64-18-6 HCO2H

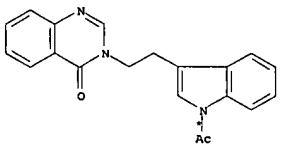
RX(12) OF 205 ...X + G ===> AB



X G

(12)

L2 ANSWER 28 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AB

RX(12) RCT X 60941-86-8, G 108-24-7
PRO AB 95274-46-7
SOL 108-24-7 Ac2O

L2 ANSWER 29 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 97:6148 CASREACT
TITLE: Indole derivatives and their medicinal use
INVENTOR(S): Coates, I. H.; Dowle, M. D.; Mills, K.; Bays, D. E.; Webb, C. F.
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Belg., 82 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

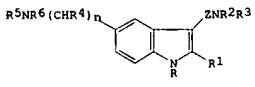
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 889931	A1	19820211	BE 1981-205644	19810811
DK 8103572	A	19820213	DK 1981-3572	19810811
DK 157995	B	19900312		
DK 157995	C	19900806		
SE 8104783	A	19820213	SE 1981-4783	19810811
SE 454777	B	19880530		
SE 454777	C	19880922		
AU 8173995	A	19820218	AU 1981-73995	19810811
AU 550010	B2	19860227		
FR 2488606	A1	19820219	FR 1981-15515	19810811
FR 2488606	B1	19841026		
NL 8103764	A	19820301	NL 1981-3764	19810811
GB 2083463	A	19820324	GB 1981-24478	19810811
GB 2083463	B	19840510		
DE 3131752	A1	19820616	DE 1981-3131752	19810811
DE 3131752	C2	19920423		
ES 504694	A1	19821101	ES 1981-504694	19810811
ZA 8105541	A	19830330	ZA 1981-5541	19810811
CH 652394	A5	19851115	CH 1981-5161	19810811
JP 57059865	A	19820410	JP 1981-125413	19810812
JP 01048896	B	19891020		
CA 1165765	A1	19840417	CA 1981-383680	19810812
ES 513934	A1	19840601	ES 1982-513934	19820713
US 4672067	A	19870609	US 1984-625648	19840628
US 4636521	A	19870113	US 1984-626383	19840629
AT 8403184	A	19860315	AT 1984-3184	19841008
AT 381491	B	19861027		
US 4839377	A	19890613	US 1987-82132	19870806

PRIORITY APPLN. INFO.:

GB 1980-26287	19800812
GB 1980-26288	19800812
AT 1981-3528	19810811
US 1981-291997	19810811
US 1981-292022	19810811
US 1981-292023	19810811
US 1982-404872	19820803
US 1982-431597	19820930
US 1983-461278	19830126
US 1985-711152	19850313

OTHER SOURCE(S): MARPAT 97:6148
GI

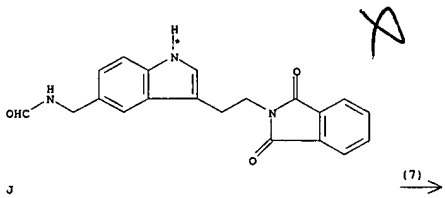
L2 ANSWER 29 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



I

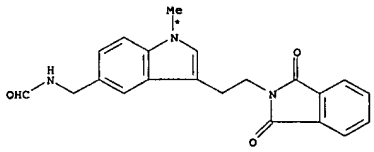
AB I [R, R1, R2, R4, R6 = H, alkyl; R3 = H, alkyl, cycloalkyl, alkenyl, aralkyl; R5 = CHO, acyl, esterified CO2H, (un)substituted carbamoyl, thiocarbamoyl, sulfamoyl; n = 0, 1; Z = alkylene, mono- or dialkylalkylene; or NR2R3 form a heterocycle or R2R3 = aralkylidene] were prepared and they are useful as antihypertensives (no data, formulations are given). 5-(Aminomethyl)-3-(2-phthalimidoethyl)indole reacted with Ac2O, and the product was hydrazinolyzed to give 5-(acetamidomethyl)-3-(2-aminoethyl)indole.

RX(7) OF 9 J ===> K



J

(7)



K

RX(7) RCT J 82017-03-6
PRO K 82017-04-7

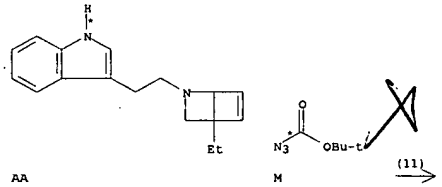
L2 ANSWER 29 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

L2 ANSWER 30 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 94:47067 CASREACT
TITLE: Synthesis and reactions of N-protected 2-lithiated pyrroles and indoles. The tert-butoxycarbonyl substituent as a protecting group
AUTHOR(S): Hasan, Iltifat; Marinelli, Edmund R.; Lin, Li-Ching Chang; Fowler, Frank W.; Levy, Alan B.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794, USA
SOURCE: Journal of Organic Chemistry (1981), 46(1), 157-64
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

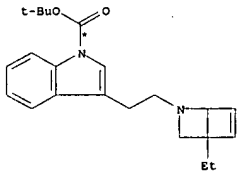
AB N-(tert-Butoxycarbonyl)pyrrole and N-tert-(butoxycarbonyl)indole were prepared and lithiated at C-2 with lithium 2,2,6,6-tetramethylpiperidide and Me3CLi, resp. The lithium reagents react with a variety of electrophiles to give C-2 substituted N-(tert-butoxycarbonyl)pyrroles and N-(tert-butoxycarbonyl)indoles. The tert-butoxycarbonyl group may be removed rapidly and in high yield from the pyrrole derivs. under basic conditions. For the indole derivs., the protecting group may be removed either with acidic or basic conditions.

RX(11) OF 14 AA + M ===> AB



AA M

L2 ANSWER 30 OF 31 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



AB
YIELD 97%

RX(11) RCT AA 343227-24-7, M 1070-19-5
PRO AB 75400-70-3

L2 ANSWER 31 OF 31 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 92:215199 CASREACT
TITLE: New method for the N-alkylation of indoles
AUTHOR(S): Suvorov, N. N.; Plutitskii, D. N.; Smushkevich, Yu. I.
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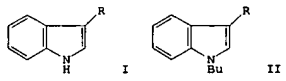
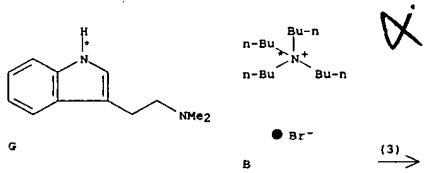
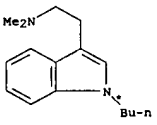


AB Treatment of indole I (R = H, Me, CH2CH2NMe2) with Bu4N+Br- in sulfolane containing K2CO3 at 170° for 3 h gave N-butylindoles II. Substitution in the 2 position of the indole ring prevented N-alkylation due to steric hindrance. 1-Butyl-N,N-dimethyltryptamine was prepared similarly.
Skatole was heated similarly to give N-butylskatol.

RX(3) OF 3 G + B ===> H



G B



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